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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 JAN 17 Pre-1988 INPI data added to MARPAT  
NEWS 4 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist  
visualization results  
NEWS 5 FEB 22 The IPC thesaurus added to additional patent databases on STN  
NEWS 6 FEB 22 Updates in EPFULL; IPC 8 enhancements added  
NEWS 7 FEB 27 New STN AnaVist pricing effective March 1, 2006  
NEWS 8 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes  
NEWS 9 MAR 08 X.25 communication option no longer available after June 2006  
NEWS 10 MAR 22 EMBASE is now updated on a daily basis  
NEWS 11 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL  
NEWS 12 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC  
thesaurus added in PCTFULL  
NEWS 13 APR 04 STN AnaVist \$500 visualization usage credit offered  
NEWS 14 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced  
NEWS 15 APR 12 Improved structure highlighting in FQHIT and QHIT display  
in MARPAT  
NEWS 16 APR 12 Derwent World Patents Index to be reloaded and enhanced during  
second quarter; strategies may be affected  
NEWS 17 MAY 10 CA/CAPLUS enhanced with 1900-1906 U.S. patent records  
NEWS 18 MAY 11 KOREAPAT updates resume  
  
NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT  
<http://download.cas.org/express/v8.0-Discover/>  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
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\* \* \* \* \*

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In an effort to enhance your experience with STN, we would  
like to better understand what you find useful. Please take  
approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: <http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW>

Thank you in advance for your participation.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:54:15 ON 16 MAY 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:54:24 ON 16 MAY 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 MAY 2006 HIGHEST RN 884382-45-0

DICTIONARY FILE UPDATES: 15 MAY 2006 HIGHEST RN 884382-45-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

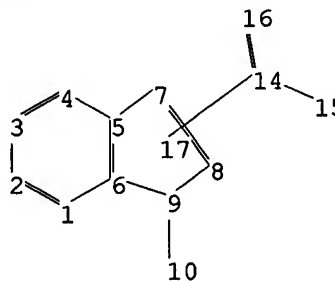
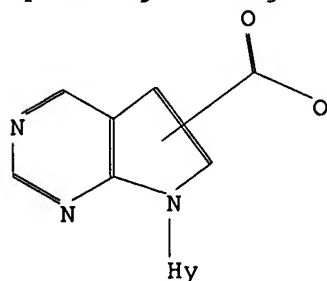
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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chain nodes :  
10 14 15 16  
ring nodes :  
1 2 3 4 5 6 7 8 9  
chain bonds :  
9-10 14-16 14-15  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9  
exact/norm bonds :  
5-7 6-9 7-8 8-9 9-10 14-16 14-15  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6

G1:Hy,Cb,Cy

G2:Cl,O

G3:CO2H,C(O)CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 14:CLASS  
15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> s l1 full

FULL SEARCH INITIATED 15:54:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 52422 TO ITERATE

100.0% PROCESSED 52422 ITERATIONS  
SEARCH TIME: 00.00.02

52 ANSWERS

L2 52 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 15:54:47 ON 16 MAY 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 16 May 2006 VOL 144 ISS 21

FILE LAST UPDATED: 15 May 2006 (20060515/ED)

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<http://www.cas.org/infopolicy.html>

=> s 12

=&gt; d 13 ibib abs hitstr

L3 ANSWER 1 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1220346 CAPLUS

DOCUMENT NUMBER: 143:477978

TITLE: Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation

INVENTOR(S): Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter

PATENT ASSIGNEE(S): IRM LLC, Bermuda

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005107760	A1	20051117	WO 2005-US15118	20050429
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

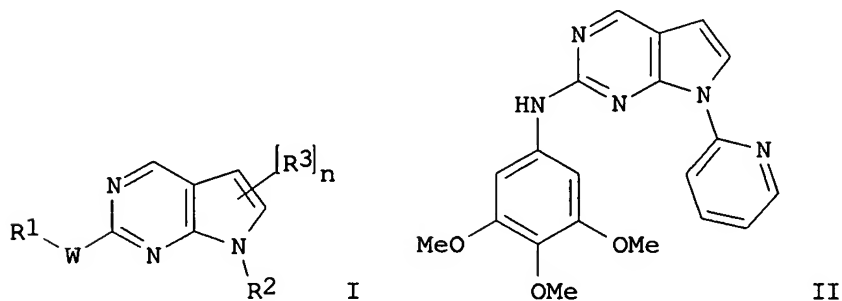
PRIORITY APPLN. INFO.:

US 2004-567346P

P 20040430

OTHER SOURCE(S): MARPAT 143:477978

GI



AB The invention provides compds. I [ $n = 0-2$ ;  $W = \text{NR}_4, \text{S}, \text{O}, \text{SO}, \text{SO}_2$  (wherein  $\text{R}_4 = \text{H}, \text{alkyl}$ );  $\text{R}_1 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$ ;  $\text{R}_2 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$ ;  $\text{R}_3 = \text{halo}, \text{OH}, \text{XSR}_5, \text{etc.}$  ( $\text{X} = \text{a bond}, \text{alkylene}$ ;  $\text{R}_5 = \text{H}, \text{alkyl}, \text{cycloalkylalkyl}$ )], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

IT 863597-79-9P 863597-80-2P

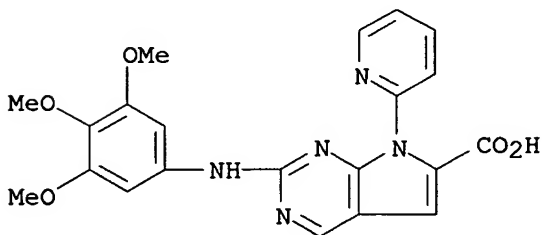
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of

keratinocyte differentiation)

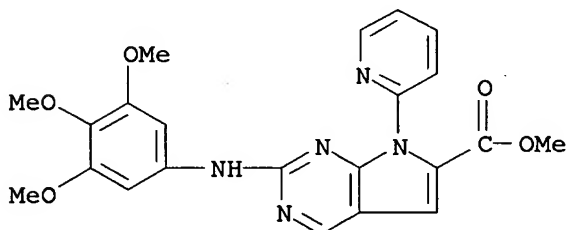
RN 863597-79-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 863597-80-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 13 ibib abs hitstr 1-65

L3 ANSWER 1 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1220346 CAPLUS

DOCUMENT NUMBER: 143:477978

TITLE: Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation

INVENTOR(S): Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter

PATENT ASSIGNEE(S): IRM LLC, Bermuda

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

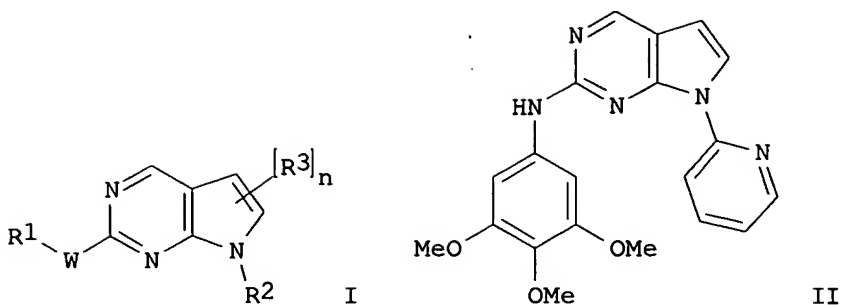
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005107760	A1	20051117	WO 2005-US15118	20050429
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2004-567346P P 20040430

OTHER SOURCE(S): MARPAT 143:477978



AB The invention provides compds. I [ $n = 0-2$ ;  $W = \text{NR}_4, \text{S}, \text{O}, \text{SO}, \text{SO}_2$  (wherein  $\text{R}_4 = \text{H}, \text{alkyl}$ );  $\text{R}_1 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$ ;  $\text{R}_2 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$ ;  $\text{R}_3 = \text{halo}, \text{OH}, \text{XSR}_5$ , etc. ( $\text{X} = \text{a bond}, \text{alkylene}$ ;  $\text{R}_5 = \text{H}, \text{alkyl}, \text{cycloalkylalkyl}$ )], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

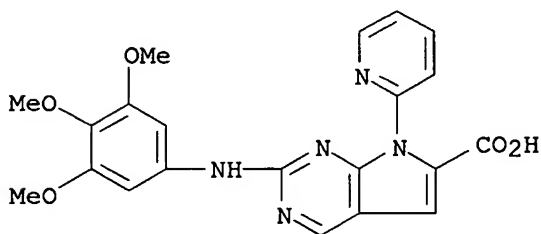
IT **863597-79-9P 863597-80-2P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation)

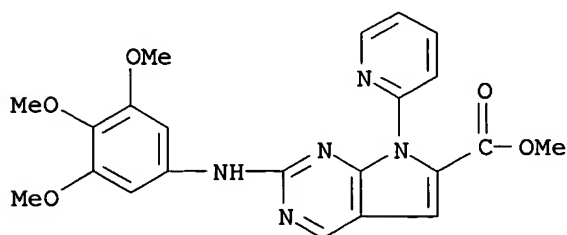
RN 863597-79-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 863597-80-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2005:962258 CAPLUS  
 DOCUMENT NUMBER: 143:266947  
 TITLE: Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors  
 INVENTOR(S): Choi, Ha-Soon; Wang, Zhicheng; Gray, Nathanael Schiander; Gu, Xiang-Ju; He, Xiaohui; He, Yun; Jiang, Tao; Liu, Yi; Richmond, Wendy; Sim, Taebo; Yang, Kunyong  
 PATENT ASSIGNEE(S): IRM LLC, Bermuda  
 SOURCE: PCT Int. Appl., 63 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080393	A1	20050901	WO 2005-US4630	20050214
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			US 2004-544944P	P 20040214
OTHER SOURCE(S):	MARPAT 143:266947			

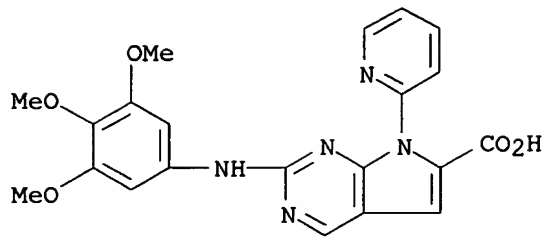
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

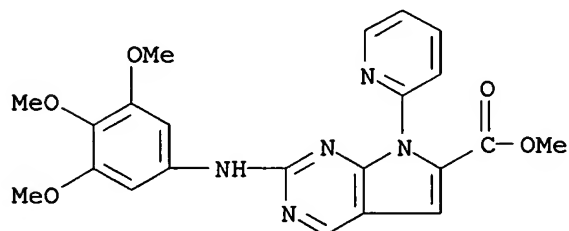
AB The invention provides a novel class of compds. I-V [n = 0-2; m = 0-3; W = NR<sub>4</sub>, S, O, SO, SO<sub>2</sub> (wherein R<sub>4</sub> = H, alkyl); R<sub>1</sub> = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R<sub>2</sub> = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R<sub>3</sub> = halo, OH, XSR<sub>5</sub>, etc. (X = a bond, alkylene; R<sub>5</sub> = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with abnormal or deregulated kinase activity, particularly diseases or disorders that involve abnormal activation of the FAK, Abl, BCR-Abl, PDGF-R, c-Kit, NPM-ALK, Flt-3, JAK2 and c-Met kinases. Over 200 compds. I-V were prepared and characterized. The preparation of the compds. I is illustrated in examples. E.g., synthesis of I [R<sub>1</sub> = 3,4,6-(MeO)<sub>3</sub>C<sub>6</sub>H<sub>2</sub>; R<sub>2</sub> = 2-pyridyl; R<sub>3</sub> = H; W = NH], starting from 5-bromo-2,4-dichloropyrimidine, was given. The compds. I-V were tested against various kinases. For example, they inhibit the enzyme activity by 50% (IC<sub>50</sub>), in a concentration of from 0.001 to 0.5 µM, especially from 0.01 to 0.1 µM.

IT **863597-79-9P 863597-80-2P**  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn of pyrrolopyrimidines and their analogs as protein kinase inhibitors)

RN 863597-79-9 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 863597-80-2 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

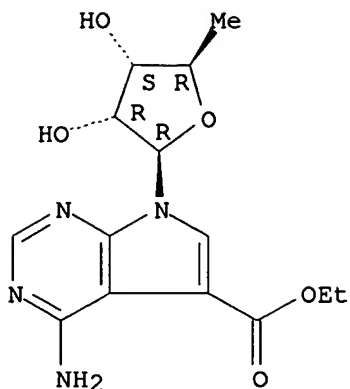
L3 ANSWER 3 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:372245 CAPLUS  
 DOCUMENT NUMBER: 143:125813  
 TITLE: QSAR studies on adenosine kinase inhibitors  
 AUTHOR(S): Agrawal, Vijay K.; Singh, Kamana; Khadikar, Padmakar V.  
 CORPORATE SOURCE: QSAR and Computer Chemical Laboratories, A.P.S. University, Rewa, 486 003, India  
 SOURCE: Medicinal Chemistry Research (2004), 13(6/7), 479-496  
 CODEN: MCREEB; ISSN: 1054-2523  
 PUBLISHER: Birkhaeuser Boston  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The present study reports QSAR study on adenosine kinase inhibitors pyrrolo[2,3-d] pyrimidine nucleoside analogs. The equalized electronegativity along with a large pool of topol. indexes are used for the purpose. The regression anal. has shown that equalized electronegativity is a good parameter which in combination with topol. indexes and an indicator parameter gave excellent model.

IT 144928-02-9  
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)  
 (QSAR studies on adenosine kinase inhibitors)

RN 144928-02-9 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:216597 CAPLUS

DOCUMENT NUMBER: 142:291323

TITLE: Compositions and methods for the treatment of severe acute respiratory syndrome (SARS)

INVENTOR(S): Hardee, Greg; Dellamary, Luis

PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020885	A2	20050310	WO 2004-US16196	20040521
WO 2005020885	A3	20050804		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2003-472774P P 20030521

AB The invention provides compns. and methods for treating a coronavirus infection, especially a SARS CoV infection. The compns. comprise an antiviral nucleoside or mimetic thereof, or an antiviral antisense agent, in a form suitable for pulmonary or nasal delivery. The methods comprise administration to a patient in need thereof the effective amount of an antiviral composition by pulmonary or nasal instillation.

IT 124738-85-8 443642-56-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

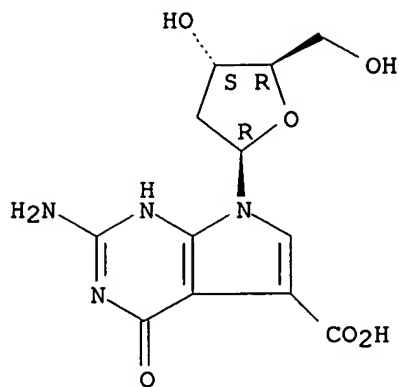
(Biological study); USES (Uses)

(compns. and methods for treatment of severe acute respiratory syndrome)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

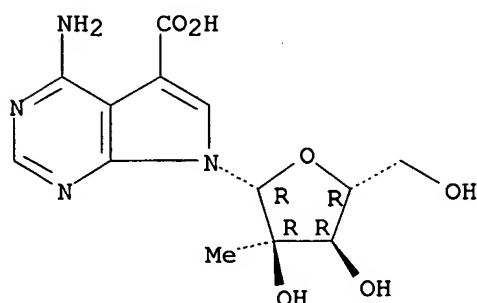
Absolute stereochemistry.



RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-beta-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 5 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:199486 CAPLUS

DOCUMENT NUMBER: 142:441277

TITLE: QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices

AUTHOR(S): Gonzalez-Diaz, Humberto; Cruz-Monteagudo, Maykel; Vina, Dolores; Santana, Lourdes; Uriarte, Eugenio; De Clercq, Erik

CORPORATE SOURCE: Department of Organic Chemistry, Faculty of Pharmacy, University of Santiago de Compostela, 15782, Spain

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(6), 1651-1657

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The unified representation of spectral moments, classic topol. indexes, quadratic indexes, and stochastic mol. descriptors show that all these mol. descriptors lie within the same family. Consequently, the same prior probability for a successful quant. structure-activity relation (QSAR) may be expected irresp. of which indexes are selected. Herein, we used stochastic spectral moments as mol. descriptors to seek a QSAR using a database of 221 bioactive compds. previously tested against diverse RNA viruses and 402 nonactive ones. The QSAR model thus obtained correctly classifies 90.9% of compds. in training. The model also correctly classifies a total of 87.9% of 207 compds. on addnl. external predicting series, 73 of them having anti-RNA-virus activity and 134 nonactive ones. In addition, all compds. were regrouped into five different subsets for leave-group-out studies: (1) anti-influenza, (2) anti-picornavirus, (3) anti-paramyxovirus, (4) anti-RSV/anti-influenza, and (5) broad range

anti-RNA-virus activity. The model has retained overall accuracies of about 90% on these studies validating model robustness. Finally, we exemplify the practical use of the model with the discovery of compds. 124 and 128. These compds. presented MIC50 values = 3.2 and 8 µg/mL against respiratory syncytial virus (RSV) resp. Both compds. also have low cytotoxicity expressed by their Minimal Cytotoxic Concns. >400 µg/mL for HeLa cells. The present approach represents an effort toward a formalization and application of mol. indexes in bioorg. and medicinal chemical

IT 81645-08-1 851071-69-7 851071-70-0

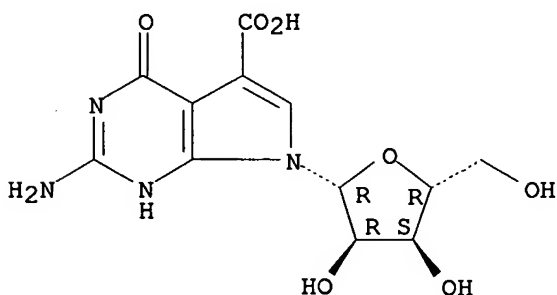
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

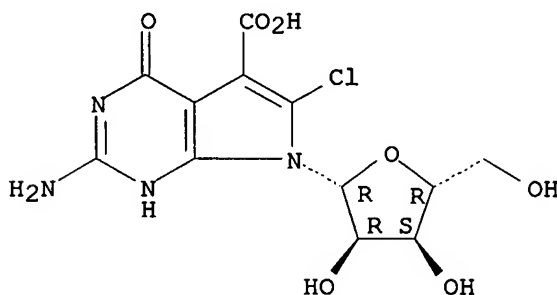
Absolute stereochemistry.



RN 851071-69-7 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-6-chloro-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

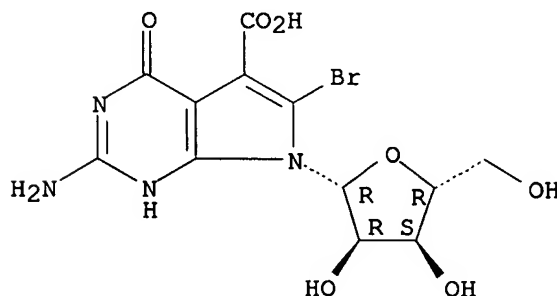
Absolute stereochemistry.



RN 851071-70-0 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-6-bromo-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 6 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:773084 CAPLUS

DOCUMENT NUMBER: 141:388156

TITLE: Structure-Activity Relationship of Heterobase-Modified 2'-C-Methyl Ribonucleosides as Inhibitors of Hepatitis C Virus RNA Replication

AUTHOR(S): Eldrup, Anne B.; Prhavic, Marija; Brooks, Jennifer; Bhat, Balkrishen; Prakash, Thazha P.; Song, Quanlai; Bera, Sanjib; Bhat, Neelima; Dande, Prasad; Cook, P. Dan; Bennett, C. Frank; Carroll, Steven S.; Ball, Richard G.; Bosserman, Michele; Burlein, Christine; Colwell, Lawrence F.; Fay, John F.; Flores, Osvaldo A.; Getty, Krista; LaFemina, Robert L.; Leone, Joseph; MacCoss, Malcolm; McMasters, Daniel R.; Tomassini, Joanne E.; Von Langen, Derek; Wolanski, Bohdan; Olsen, David B.

CORPORATE SOURCE: Department of Medicinal Chemistry, Isis Pharmaceuticals, Carlsbad, CA, 92008, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(21), 5284-5297

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:388156

AB Hepatitis C virus infection constitutes a significant health problem in need of more effective therapies. The authors have recently identified 2'-C-methyladenosine and 2'-C-methylguanosine as potent nucleoside inhibitors of HCV RNA replication in vitro. However, both of these compds. suffered from significant limitations. 2'-C-Methyladenosine was found to be susceptible to enzymic conversions by adenosine deaminase and purine nucleoside phosphorylase, and it displayed limited oral bioavailability in the rat. 2'-C-Methylguanosine, on the other hand, was neither efficiently taken up in cells nor phosphorylated well. As part of an attempt to address these limitations, the authors now report upon the synthesis and evaluation of a series of heterobase-modified 2'-C-Me ribonucleosides. The structure-activity relationship within this series of nucleosides reveals 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine and 4-amino-5-fluoro-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine as potent and noncytotoxic inhibitors of HCV RNA replication. Both 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine and 4-amino-5-fluoro-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine display improved enzymic stability profiles as compared to that of 2'-C-methyladenosine. Consistent with these observations, the most potent compound, 4-amino-5-fluoro-7H-pyrrolo[2,3-d]pyrimidine ribonucleoside, is orally bioavailable in the rat. Together, the potency of the 2'-C-methyl-4-amino-pyrrolo[2,3-d]pyrimidine ribonucleosides and their improved pharmacokinetic properties relative to that of 2'-C-methyladenosine suggests that this class of compds. may have clin. utility.

IT 443642-56-6P

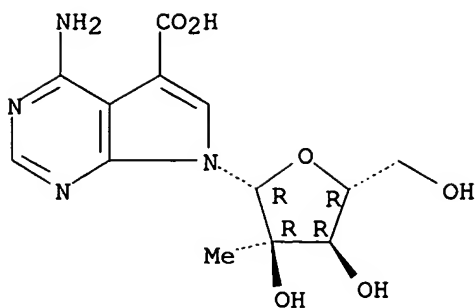
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structure-activity relationship of heterobase-modified 2'-C-Me ribonucleosides as inhibitors of hepatitis C virus RNA replication)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:403777 CAPLUS

DOCUMENT NUMBER: 141:169851

TITLE: A TOPS-MODE approach to predict adenosine kinase inhibition

AUTHOR(S): Gonzalez, Maykel Perez; Moldes, Maria del Carmen Teran

CORPORATE SOURCE: Service Unit, Experimental Sugar Cane Station 'Villa Clara-Cienfuegos', Villa Clara, C.P. 53100, Cuba

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(12), 3077-3079

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The TOPol. Sub-Structural Mol. Design (TOPS-MODE) approach has been used to address the adenosine kinase inhibitory activity of pyrrolo[2,3-d]pyrimidine nucleoside analogs. A model capable of describing around 77% of the variance in exptl. activity of 32 analogs was developed on the basis of this approach. In contrast, out of nine different approaches, including the use of Constitutional, Topol., BCUT, 2D autocorrelations, geometrical, RDF, 3D Morse, WHIM, and GETAWAY descriptors none were able to explain more than 70% of the variance in the above-mentioned property with the same number of descriptors. Although statistically significant models were derived containing descriptors other than spectral moments, the model that exhibited the best fit was based on these variables.

IT 144928-02-9

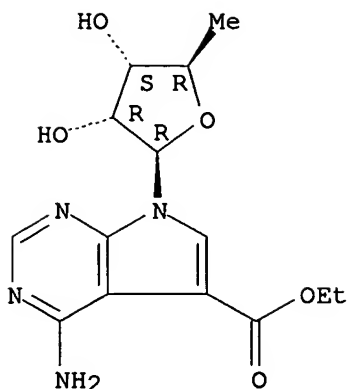
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(TOPS-MODE approach permits QSAR anal. of adenosine kinase inhibition by pyrrolo[2,3-d]pyrimidine nucleoside analogs)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:951160 CAPLUS

DOCUMENT NUMBER: 140:13688

TITLE: Oligonucleotides having modified nucleoside units with various linkages, and their uses as antisense agents, ribozymes, aptamers, siRNA, probes, and primers, or when hybridized to RNA, as substrates for RNA cleaving enzymes

INVENTOR(S): Eldrup, Anne; Cook, Phillip Dan; Parshall, Lynne B.

PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 161 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003100017	A2	20031204	WO 2003-US16526	20030523
WO 2003100017	A3	20040826		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003241621	A1	20031212	AU 2003-241621	20030523
US 2004014108	A1	20040122	US 2003-444298	20030523
PRIORITY APPLN. INFO.:			US 2002-383358P	P 20020524
			WO 2003-US16526	W 20030523

OTHER SOURCE(S): MARPAT 140:13688

AB Disclosed are oligonucleotides that include one or more modified nucleoside units. The examples present the representative preparation of modified nucleosides and nucleoside amidites, for incorporation into said oligonucleotides. The oligonucleotides are particularly useful as antisense agents, ribozymes aptamer, siRNA agents, probes and primers or, when hybridized to an RNA, as a substrate for RNA cleaving enzymes including Rnase H and dsRNase.

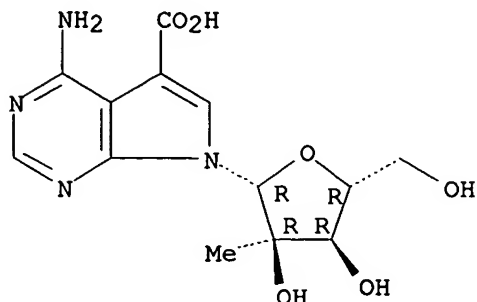
IT 443642-56-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of modified nucleosides and nucleoside amidites for incorporation into oligonucleotides, and uses)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 9 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:951042 CAPLUS

DOCUMENT NUMBER: 140:24085

TITLE: Oligonucleotides having modified nucleoside units with various linkages, and their uses as antisense agents, ribozymes, aptamers, siRNA, probes, and primers, or when hybridized to RNA, as substrates for RNA cleaving enzymes

INVENTOR(S): Eldrup, Anne; Cook, Phillip Dan; Parshall, B. Lynne

PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 271 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099840	A1	20031204	WO 2003-US16502	20030523
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003237249	A1	20031212	AU 2003-237249	20030523
US 2004014957	A1	20040122	US 2003-444628	20030523
PRIORITY APPLN. INFO.:			US 2002-383438P	P 20020524
			WO 2003-US16502	W 20030523

OTHER SOURCE(S): MARPAT 140:24085

AB Disclosed are oligonucleotides that include one or more modified nucleoside units. The examples present the representative preparation of modified nucleosides and nucleoside amidites, for incorporation into said oligonucleotides. The oligonucleotides are particularly useful as antisense agents, ribozymes aptamer, siRNA agents, probes and primers or, when hybridized to an RNA, as a substrate for RNA cleaving enzymes including Rnase H and dsRNase.

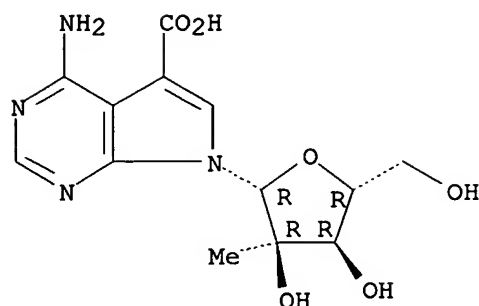
IT 443642-56-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(oligonucleotides having modified nucleoside units with various linkages)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:681321 CAPLUS

DOCUMENT NUMBER: 140:246064

TITLE: Quantitative Structure-Activity Relationship Study of 5-Iodo- and Diaryl-analogues of Tubercidin: Inhibitors of Adenosine Kinase

AUTHOR(S): Singh, P.; Kumar, Rajesh; Sharma, B. K.

CORPORATE SOURCE: Dep. Chem., S.K. Government Coll., Sikar, 332 001, India

SOURCE: Journal of Enzyme Inhibition and Medicinal Chemistry (2003), 18(5), 395-402

CODEN: JEIMAZ; ISSN: 1475-6366

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The adenosine kinase inhibitory (AKI) activity of 5-iodo and diaryl analogs of tubercidin is quant. analyzed using Fujita-Ban and Hansch type analyses. The Fujita-Ban anal. being a non-parametric approach assigned the highest contribution to Cl at the X-position, C6H4-4-Cl, C6H5, 2-furanyl and I at the Y-position and CH2NH2 and CH3 at the Z-position. In addition, a OH substituent at the C-position also emerged as a better choice possibly due to its engagement in hydrogen bonding with some active site function. Thus a compound having Cl, C6H4-4-Cl, CH2NH2 and OH resp. at X-, Y-, Z- and C-positions is predicted to have a potency nearly 1.5 orders of magnitude higher than the most potent compound of the parent data set. The Hansch type anal., on the other hand, is a parametric approach and is carried out on two sub-sets of original compds. This sub-division is based on size and nature of the substituents present at the X- and Y-positions. For the compds. in the first sub-set the derived significant correlation equation suggested that the substituent at the Y-position exhibiting a higher field effect and a substituent such as Cl and CH2NH2 at X- and Z-positions, resp., are important for a compound to show increased AKI activity. Thio/alkylthio at X and CH2OCH3 at Z, on the other hand, lead to a detrimental effect. Similarly for the compds. in the second sub-set, the derived significant correlation equation showed that a substituent at the X-position having a higher neg. field effect, a substituent at the Y-position having bulky groups and the C-position occupied by a OH group are essential for enhancement of the activity of a compound

IT 144928-02-9

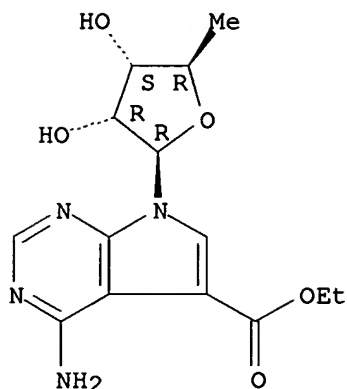
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(quant. structure-activity relationship study of 5-iodo- and diaryl-analogs of tubercidin as inhibitors of adenosine kinase)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:656596 CAPLUS

DOCUMENT NUMBER: 139:191380

TITLE: Methods of inhibiting orthopoxvirus replication with nucleoside compounds

INVENTOR(S): Olsen, David B.; Lafemina, Robert L.; Eldrup, Anne B.; Bera, Sanjib

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 99 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003068244	A1	20030821	WO 2003-US3703	20030207
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2474563	AA	20030821	CA 2003-2474563	20030207
AU 2003209045	A1	20030904	AU 2003-209045	20030207
EP 1476169	A1	20041117	EP 2003-707772	20030207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005164960	A1	20050728	US 2003-504445	20030207
JP 2005527499	T2	20050915	JP 2003-567425	20030207
PRIORITY APPLN. INFO.:			US 2002-356805P	P 20020213
			WO 2003-US3703	W 20030207

OTHER SOURCE(S): MARPAT 139:191380

AB The present invention provides methods of inhibiting orthopoxvirus replication and/or treating orthopoxvirus infection with certain nucleoside compds. and derivs. thereof. These compds. are particularly useful as inhibitors of vaccinia virus and variola virus replication and/or for the treatment of vaccinia virus and variola virus infection. The nucleoside compds. may be administered alone or in combination with other agents active against orthopoxvirus infection, in particular against vaccinia virus or variola virus infection. Another aspect of the present invention provides for the use of such nucleoside compds. in the manufacture of a medicament for the inhibition of orthopoxvirus replication and/or for

the treatment of orthopoxvirus infection. Yet a further aspect of the present invention provides such nucleoside compds. for use as a medicament for the inhibition of orthopoxvirus replication and/or for the treatment of orthopoxvirus infection.

IT 443642-56-6P

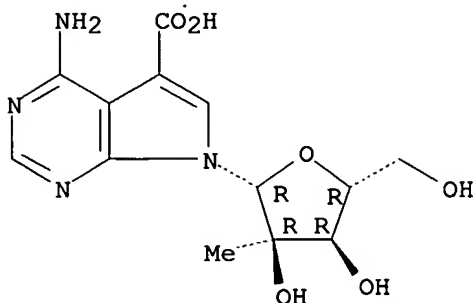
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(inhibiting orthopoxvirus replication with nucleoside compds.)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:590940 CAPLUS

DOCUMENT NUMBER: 139:133787

TITLE: Preparation of deazapurine nucleoside analogs as antiviral agents

INVENTOR(S): An, Haoyun; Ding, Yili; Chamakura, Varaprasad; Hong, Zhi

PATENT ASSIGNEE(S): Ribapharm Inc., USA

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

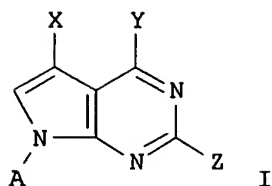
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003061576	A2	20030731	WO 2003-US1545	20030117
WO 2003061576	A3	20040401		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2002-350296P P 20020117

OTHER SOURCE(S): MARPAT 139:133787

GI



AB Methods, compns., and uses for various deazapurine nucleoside libraries and library compds. I are provided. Particularly preferred deazapurine nucleosides include 7-deazapurine nucleosides, 7-deaza-8-azapurine nucleosides, toyocamycin nucleoside analogs, 3-deazapurine nucleosides, and 9-deazapurine nucleosides, while preferred uses especially include use of such compds. as pharmacol., and particularly antiviral agents. 4-N,N-dimethylamino-7-( $\beta$ -D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine-5-N-hydroxycarbamide was prepared and tested in vitro as antiviral agent.

IT 565455-12-1P 565455-13-2P 565455-22-3P

565455-23-4DP, resin bound 565455-23-4P

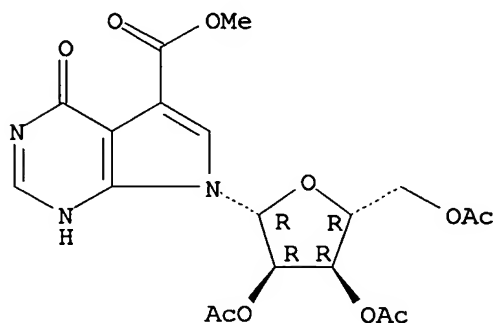
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of deazapurine nucleoside analogs as antiviral agents)

RN 565455-12-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-(2,3,5-tri-O-acetyl- $\beta$ -D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

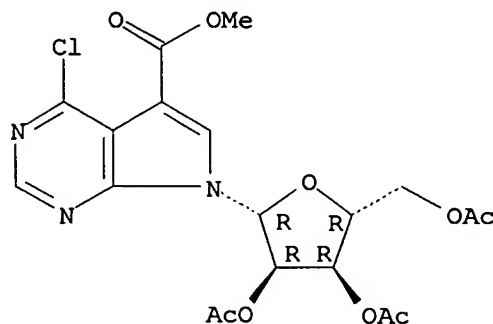
Absolute stereochemistry.



RN 565455-13-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-(2,3,5-tri-O-acetyl- $\beta$ -D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

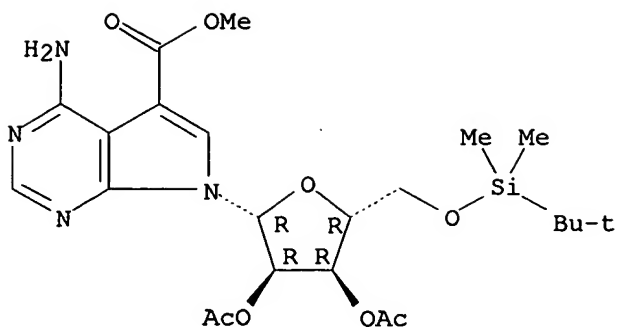
Absolute stereochemistry.



RN 565455-22-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]- $\beta$ -D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

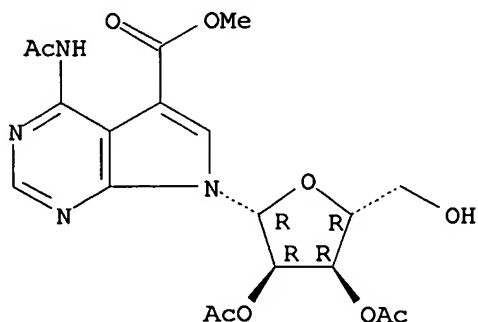
Absolute stereochemistry.



RN 565455-23-4 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-beta-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

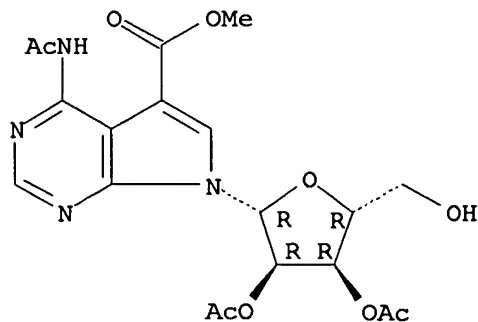
Absolute stereochemistry.



RN 565455-23-4 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-beta-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 13 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:506580 CAPLUS

DOCUMENT NUMBER: 139:79178

TITLE: Synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivatives and use as phosphodiesterase VII inhibitors and in combination with other agents

INVENTOR(S): Eggenweiler, Hans-Michael; Wolf, Michael

PATENT ASSIGNEE(S): Merck Patent GmbH, Germany

SOURCE: Ger. Offen., 36 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10163991	A1	20030703	DE 2001-10163991	20011224
CA 2471538	AA	20030710	CA 2002-2471538	20021108
WO 2003055882	A1	20030710	WO 2002-EP12533	20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002367090	A1	20030715	AU 2002-367090	20021108
EP 1458722	A1	20040922	EP 2002-805744	20021108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002015308	A	20041221	BR 2002-15308	20021108
CN 1608067	A	20050420	CN 2002-826034	20021108
JP 2005520801	T2	20050714	JP 2003-556412	20021108
US 2005059686	A1	20050317	US 2004-500040	20040623
ZA 2004005859	A	20050517	ZA 2004-5859	20040722
PRIORITY APPLN. INFO.:			DE 2001-10163991	A 20011224
			WO 2002-EP12533	W 20021108

OTHER SOURCE(S): MARPAT 139:79178

AB The invention concerns the synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs., their physiol. acceptable salts, stereoisomers, solvates, mixts. thereof and their use as phosphodiesterase VII inhibitors in the treatment of diseases that are influenced by the phosphodiesterase VII regulation of human eosinophil activation and degranulation. Osteoporesis, tumors, cachexia, atherosclerosis, rheumatoid arthritis, multiple sclerosis, diabetes mellitus, AIDS, autoimmune and heart diseases can be treated with the drugs. Thus the synthesis of 5-isopropyl-4-oxo-7-p-tolyl-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid Et ester and analog compds. is described along with injection, suppository, tablet and other formulations.

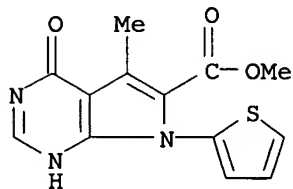
IT **552298-62-1P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs. and use as phosphodiesterase VII inhibitors and in combination with other agents)

RN 552298-62-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-(2-thienyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 14 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:491245 CAPLUS

DOCUMENT NUMBER: 139:53258

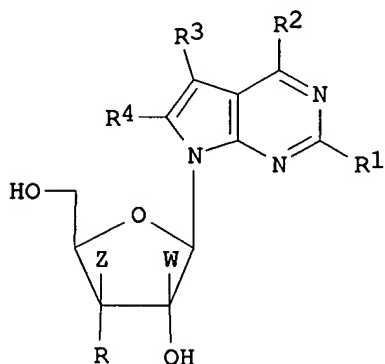
TITLE: Solid phase synthesis and combinatorial libraries of deazapurine nucleosides useful in the treatment of viral infections and neoplastic diseases

INVENTOR(S): Girardet, Jean-Luc; An, Haoyun; Chamakura, Varaprasad; Gunic, Esmir; Hong, Zhi

PATENT ASSIGNEE(S): Ribapharm Inc., USA

SOURCE: PCT Int. Appl., 59 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051899	A1	20030626	WO 2002-US40416	20021217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002353165	A1	20030630	AU 2002-353165	20021217
PRIORITY APPLN. INFO.:			US 2001-342410P	P 20011217
			WO 2002-US40416	W 20021217
OTHER SOURCE(S):		MARPAT 139:53258		
GI				



I

AB Deazapurine nucleoside analogs I, wherein R is H, OH; R1-R4 are independently H, halogen, NH2, NHR', R', CN, CONH2, N3, CH2CN; R' is substituted alkyl, unsubstituted alkyl, substituted aryl, and an unsubstituted aryl; W and Z are independently hydrogen, N3, NH2, OH, SH, R5, or NHR5 wherein R5 is an alkyl, substituted alkyl, alkenyl, a substituted alkenyl, alkynyl, substituted alkynyl, aryl, substituted aryl; are prepared in a combinatorial library approach. Particularly preferred compds. and libraries include various 7-deazapurines, 9-deazapurines, and 7-deaza-8-azaguanosine as heterocyclic bases, and it is generally preferred that such nucleosides include a ribofuranose as the sugar moiety. It is further contemplated that compds. generated using contemplated libraries may be useful in the treatment of various conditions, particularly viral infections and neoplastic diseases (no data). Thus, I (R = OH; R1 = R4 = Z = W = H; R2 = NHBn; R3 = Ph) was prepared useful in the treatment of viral infections and neoplastic diseases.

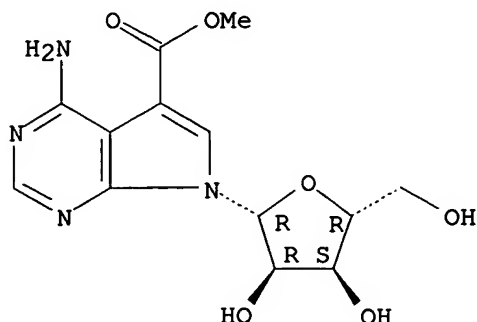
IT 18440-68-1P 547754-20-1P 547754-21-2P  
 547754-22-3P 547754-23-4DP, 4-methoxytrityl resin  
 support 547754-23-4P 547754-24-5DP, 4-methoxytrityl  
 resin support 547754-37-0P 547754-38-1DP,  
 4-methoxytrityl resin support 547754-38-1P 547754-39-2DP  
 , 4-methoxytrityl resin support  
 RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT  
 (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant  
 or reagent)

(solid phase synthesis and combinatorial libraries of deazapurine nucleosides useful in treatment of viral infections and neoplastic diseases)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7- $\beta$ -D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

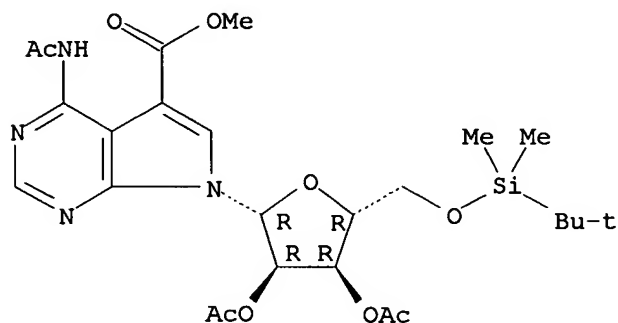
Absolute stereochemistry.



RN 547754-20-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]- $\beta$ -D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

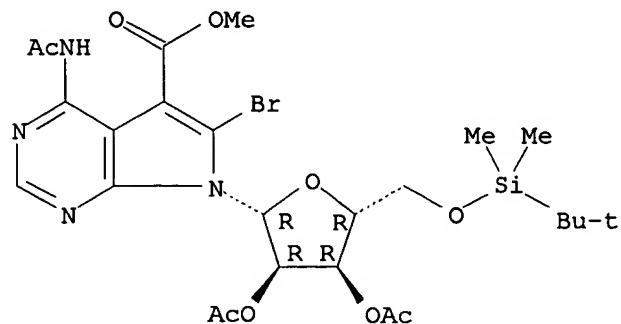
Absolute stereochemistry.



RN 547754-21-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-6-bromo-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]- $\beta$ -D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

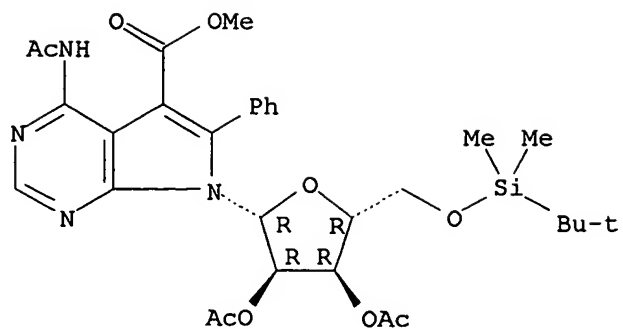
Absolute stereochemistry.



RN 547754-22-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]- $\beta$ -D-ribofuranosyl]-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

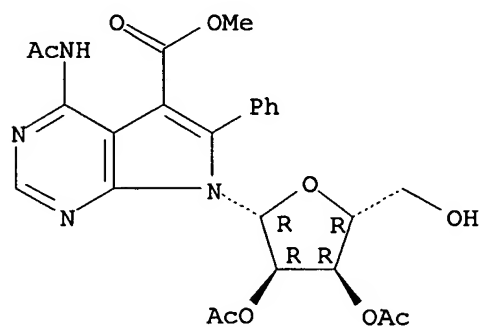
Absolute stereochemistry.



RN 547754-23-4 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl- $\beta$ -D-ribofuranosyl)-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

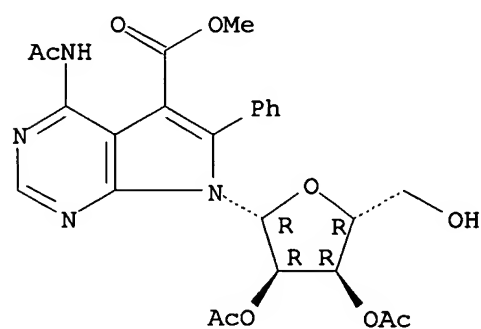
Absolute stereochemistry.



RN 547754-23-4 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl- $\beta$ -D-ribofuranosyl)-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

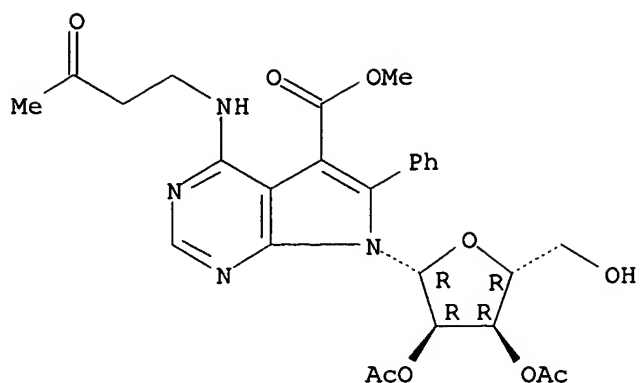
Absolute stereochemistry.



RN 547754-24-5 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-(2,3-di-O-acetyl- $\beta$ -D-ribofuranosyl)-4-[(3-oxobutyl)amino]-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

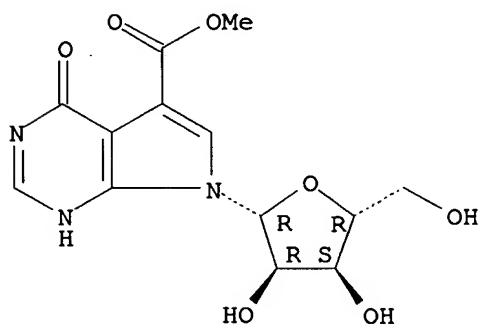
Absolute stereochemistry.



RN 547754-37-0 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

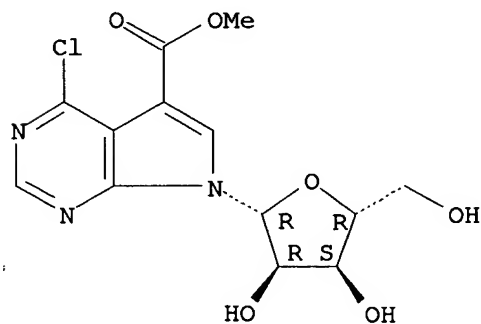
Absolute stereochemistry.



RN 547754-38-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

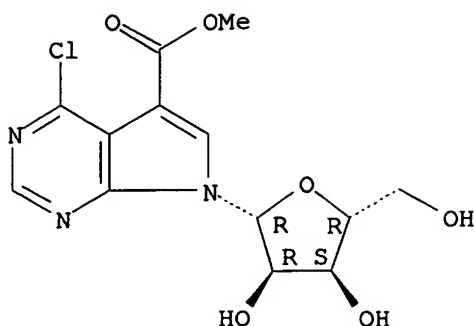
Absolute stereochemistry.



RN 547754-38-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

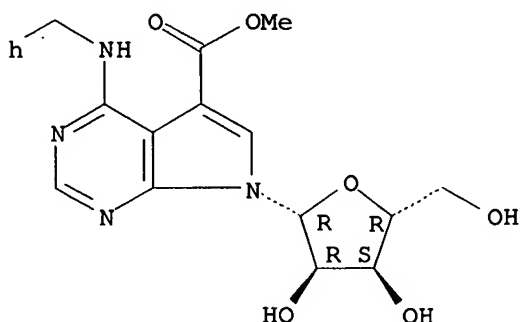
Absolute stereochemistry.



RN 547754-39-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-[(phenylmethyl)amino]-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:202427 CAPLUS

DOCUMENT NUMBER: 138:221789

TITLE: Preparation of dioxolane and oxathiolane nucleosides as antivirals and inhibitors of RNA-dependent RNA viral polymerase

INVENTOR(S): Carroll, Steven S.; MacCoss, Malcolm; Kuo, Lawrence C.; Olsen, David B.; Bhat, Balkrishen; Eldrup, Anne Bettina; Prhavc, Marija; Malik, Leila; Bera, Sanjib

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

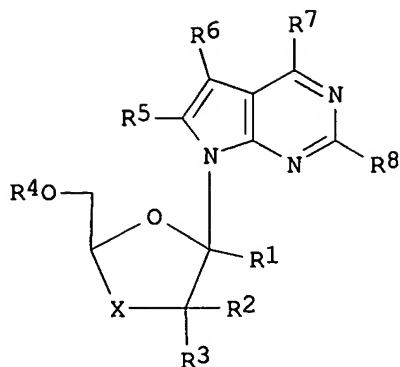
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020222	A2	20030313	WO 2002-US28078	20020829
WO 2003020222	A3	20031127		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2001-317070P P 20010904



I

AB The present invention provides 1,3-dioxolane and 1,3-oxathiolane derivs. I, wherein X is O or S(O)<sub>n</sub>; n is 0-2; R1 is hydrogen, Me, hydroxymethyl, or fluoromethyl; R2 and R3 are each independently hydrogen or alkyl, wherein alkyl is optionally substituted with hydroxy, amino, alkoxy, alkylthio, or one to three halogen atoms; R4 is H, alkylcarbonyl, phosphate; R5 is H, alkyl, alkynyl, halogen, cyano, carboxy, alkyloxycarbonyl, azido, amino, alkylamino, di(alkyl)amino, hydroxy, alkoxy, alkylthio, alkylsulfonyl, aminomethyl; R6 is hydrogen, cyano, nitro, alkyl, NHCONH<sub>2</sub>, amide, ester, C(=NH)NH<sub>2</sub>, hydroxy, alkoxy, amino, alkylamino, di(alkyl)amino, halogen, (1,3-oxazol-2-yl), (1,3-thiazol-2-yl), or (imidazol-2-yl); R7 and R8 are each independently hydrogen, hydroxy, halogen, alkoxy, amino, alkylamino, di(alkyl)amino, cycloalkylamino, or di(cycloalkyl)amino; wherein said RNA-dependent RNA viral polymerase is Flaviviridae viral polymerase or Picornaviridae viral polymerase and said RNA-dependent RNA viral replication is Flaviviridae viral replication or Picornaviridae viral replication. These compds. are also inhibitors of RNA-dependent RNA viral replication and are useful in the treatment of RNA-dependent RNA viral infection. The invention also describes pharmaceutical compns. containing such 1,3-dioxolane and 1,3-oxathiolane derivs. alone or in combination with other agents active against RNA-dependent RNA viral infection. Also disclosed are methods of inhibiting RNA-dependent RNA viral polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the compds. of the present invention. Flaviviridae viral polymerase is selected from the group consisting of hepatitis C virus polymerase, yellow fever virus polymerase, dengue virus polymerase, West Nile virus polymerase, Japanese encephalitis virus polymerase, and bovine viral diarrhea virus (BVDV) polymerase. Thus, cis-2-hydroxymethyl-4-(4-amino-5-carboxy-1H-pyrrolo[2,3-d]pyrimidin-7-yl)-1,3-dioxolane was prepared as antiviral agent and inhibitor of RNA-dependent RNA viral polymerase.

IT 501013-62-3P 501013-73-6P 501013-87-2P  
501013-98-5P

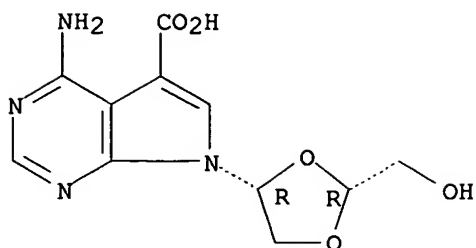
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dioxolane and oxathiolane nucleosides as antivirals and inhibitors of RNA-dependent RNA viral polymerase)

RN 501013-62-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,4R)-2-(hydroxymethyl)-1,3-dioxolan-4-yl]-, rel- (9CI) (CA INDEX NAME)

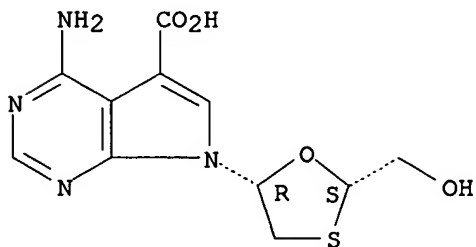
Relative stereochemistry.



RN 501013-73-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,5S)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-, rel- (9CI) (CA INDEX NAME)

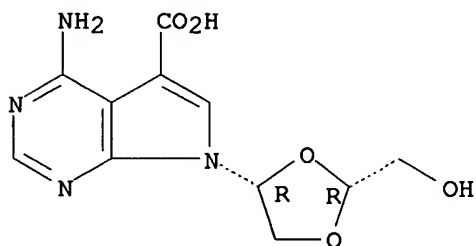
Relative stereochemistry.



RN 501013-87-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,4R)-2-(hydroxymethyl)-1,3-dioxolan-4-yl]- (9CI) (CA INDEX NAME)

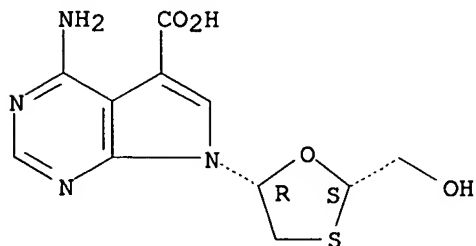
Absolute stereochemistry.



RN 501013-98-5 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2S,5R)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 16 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:555629 CAPLUS

DOCUMENT NUMBER: 137:125359

TITLE: Preparation of nucleoside derivatives as inhibitors of

INVENTOR(S):

RNA-dependent RNA viral polymerase  
Carroll, Steven S.; Lafemina, Robert L.; Hall, Dawn L.; Himmelberger, Amy L.; Kuo, Lawrence C.; Maccoss, Malcolm; Olsen, David B.; Rutkowski, Carrie A.; Tomassini, Joanne E.; An, Haoyun; Bhat, Balkrishen; Bhat, Neelima; Cook, Phillip Dan; Eldrup, Anne B.; Guinasso, Charles J.; Prhavc, Marija; Prakash, Thazha P.

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE:

PCT Int. Appl., 235 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

2

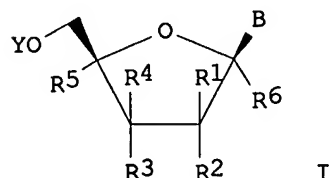
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057425	A2	20020725	WO 2002-US1531	20020118
WO 2002057425	A3	20050421		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2433878	AA	20020725	CA 2002-2433878	20020118
US 2002147160	A1	20021010	US 2002-52318	20020118
US 6777395	B2	20040817		
CN 1498221	A	20040519	CN 2002-806977	20020118
JP 2004532184	T2	20041021	JP 2002-558479	20020118
EP 1539188	A2	20050615	EP 2002-709095	20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004072788	A1	20040415	US 2003-431657	20030507
ZA 2003005078	A	20040521	ZA 2003-5078	20030630
US 2004067901	A1	20040408	US 2003-688691	20031017
US 2004110717	A1	20040610	US 2004-250873	20040116
US 2005272676	A1	20051208	US 2005-200499	20050809
PRIORITY APPLN. INFO.:				
			US 2001-263313P	P 20010122
			US 2001-282069P	P 20010406
			US 2001-299320P	P 20010619
			US 2001-344528P	P 20011025
			US 2002-52318	A3 20020118
			WO 2002-US1531	W 20020118
			US 2003-431657	B1 20030507

OTHER SOURCE(S):

MARPAT 137:125359

GI



AB The present invention provides the preparation of nucleoside compds. I, wherein B is nucleobase, Y is H, alkylcarbonyl, phosphate; R1 is H, alkenyl, alkynyl, alkyl; R2 and R3 are independently H, OH, halogen, alkyl, alkoxy, alkenyloxy, alkylthio, alkylcarbonyloxy, aryloxycrbonyl, azido, amino, alkylamino; R1 and R2 together with the carbon atom to which they are attached form a 3- to 6-membered heterocycle; R4 is H, OH, SH, NH2,

alkylamino, cycloalkylamino, halogen, alkyl, alkoxy, CF<sub>3</sub>; R<sub>5</sub> and R<sub>6</sub> are independently H, hydroxymethyl, Me, fluoromethyl; and certain derivs. thereof which are inhibitors of RNA-dependent RNA viral polymerase. These compds. are inhibitors of RNA-dependent RNA viral replication and are useful for the treatment of RNA-dependent RNA viral infection. They are particularly useful as inhibitors of hepatitis C virus (HCV) NS5B polymerase, as inhibitors of HCV replication, and/or for the treatment of hepatitis C infection. The invention also describes pharmaceutical compns. containing such nucleoside compds. alone or in combination with other agents active against RNA-dependent RNA viral infection, in particular HCV infection. Also disclosed are methods of inhibiting RNA-dependent RNA polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the nucleoside compds. of the present invention. Thus, 4-amino-1-(2-C-methyl-β-D-ribofuranosyl)-1H-pyrazolo[3,4-d]pyrimidine was prepared as inhibitors of RNA-dependent RNA viral polymerase. Representative compds. tested in the HCV NS5B polymerase assay exhibited IC's less than 100 μM. The compds. of the present invention were also evaluated for their ability to affect the replication of Hepatitis C Virus RNA in cultured hepatoma (HuH-7) cells containing a sub-genomic HCV Replicon.

IT **443642-56-6P**

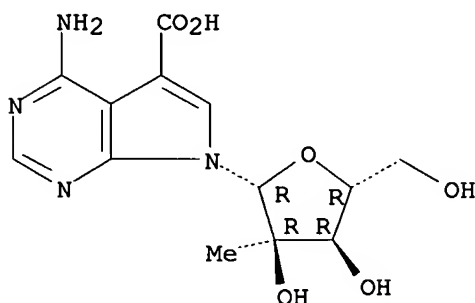
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nucleoside derivs. as inhibitors of RNA-dependent human RNA viral polymerase)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 17 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:55511 CAPLUS

DOCUMENT NUMBER: 137:109450

TITLE: Preparation of nucleoside derivatives as inhibitors of RNA-dependent RNA viral polymerase

INVENTOR(S): Carroll, Steven S.; Maccoss, Malcolm; Olsen, David B.; Bhat, Balkrishen; Bhat, Neelima; Cook, Phillip Dan; Eldrup, Anne B.; Prakash, Thazha P.; Prhavc, Marija; Song, Quanlai

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057287	A2	20020725	WO 2002-US3086	20020118
WO 2002057287	A3	20021010		

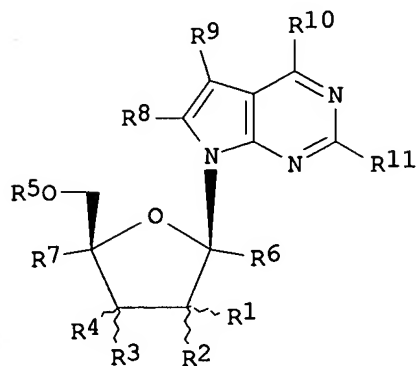
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,  
LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,  
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,  
UG, US, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,  
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2434386	AA	20020825	CA 2002-2434386	20020118
US 2002147160	A1	20021010	US 2002-52318	20020118
US 6777395	B2	20040817		
EE 200300338	A	20031015	EE 2003-338	20020118
EP 1355916	A2	20031029	EP 2002-709299	20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002006614	A	20040217	BR 2002-6614	20020118
CN 1498221	A	20040519	CN 2002-806977	20020118
JP 2004520367	T2	20040708	JP 2002-557963	20020118
NZ 526703	A	20041224	NZ 2002-526703	20020118
US 2004072788	A1	20040415	US 2003-431657	20030507
ZA 2003005078	A	20040521	ZA 2003-5078	20030630
BG 108000	A	20040831	BG 2003-108000	20030717
NO 2003003289	A	20030919	NO 2003-3289	20030721
US 2004067901	A1	20040408	US 2003-688691	20031017
US 2005272676	A1	20051208	US 2005-200499	20050809
PRIORITY APPLN. INFO.:				
			US 2001-263313P	P 20010122
			US 2001-282069P	P 20010406
			US 2001-299320P	P 20010619
			US 2001-344528P	P 20011025
			US 2002-52318	A3 20020118
			WO 2002-US3086	W 20020118
			US 2003-431657	B1 20030507

OTHER SOURCE(S): MARPAT 137:109450  
GI



I

AB The present invention provides nucleoside compds. I, wherein R1 is alkenyl, alkynyl, alkyl, wherein alkyl is unsubstituted or substituted with hydroxy, amino, alkoxy, alkylthio, one to three fluorine atoms; R2 is hydrogen, fluorine, hydroxy, mercapto, alkoxy, alkyl; or R1 and R2 together with the carbon atom to which they are attached form a 3- to 6-membered saturated monocyclic ring system optionally containing a heteroatom selected from O, S, and NC-alkyl; R3 and R4 are each independently hydrogen, cyano, azido, halogen, hydroxy, mercapto, amino, alkoxy, alkenyl, alkynyl, alkyl; R5 is hydrogen, alkylcarbonyl, phosphate; R6 and R7 are each independently hydrogen, Me, hydroxymethyl, or fluoromethyl; R8 is hydrogen, alkyl, alkynyl, halogen, cyano, carboxy, alkyloxycarbonyl, azido, amino, alkylamino, di(alkyl)amino, hydroxy, alkoxy, alkylthio, alkylsulfonyl, alkylaminomethyl, cycloheteroalkyl; R9 is hydrogen, cyano, nitro, alkyl, NHCONH2, amide, thioamide, ester, C(=NH)NH2, hydroxy, alkoxy, amino, alkylamino, di(alkyl)amino, halogen, (1,3-oxazol-2-yl), (1,3-thiazol-2-yl), or (imidazol-2-yl); R10 and R11 are each independently

hydrogen, hydroxy, halogen, alkoxy, amino, alkylamino, di(alkyl)amino, cycloalkylamino, di(cycloalkyl)amino, cycloheteroalkyl, and certain derivs. thereof which are inhibitors of RNA-dependent RNA viral polymerase. These compds. are inhibitors of RNA-dependent RNA viral replication and are useful for the treatment of RNA-dependent RNA viral infection. They are particularly useful as inhibitors of hepatitis C virus (HCV) NS5B polymerase, as inhibitors of HCV replication, and/or for the treatment of hepatitis C infection. The invention also describes pharmaceutical compns. containing such nucleoside compds. alone or in combination with other agents active against RNA-dependent RNA viral infection, in particular HCV infection. Also disclosed are methods of inhibiting RNA-dependent RNA polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the nucleoside compds. of the present invention. Thus, 4-amino-7-(2-C-methyl- $\beta$ -D-arabinofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine was prepared as inhibitors of RNA-dependent RNA viral polymerase. Representative compds. tested in the HCV NS5B polymerase assay exhibited IC's less than 100  $\mu$ M. The nucleoside derivs. were also screened for cytotoxicity against cultured hepatoma (HuH-7) cells containing a sub-genomic HCV Replicon in an MTS cell-based assay.

IT 443642-56-6P 443643-13-8P

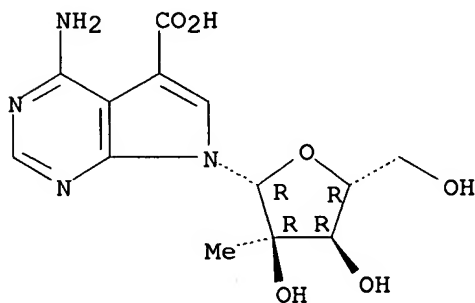
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nucleoside derivs. as inhibitors of RNA-dependent human RNA viral polymerase)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

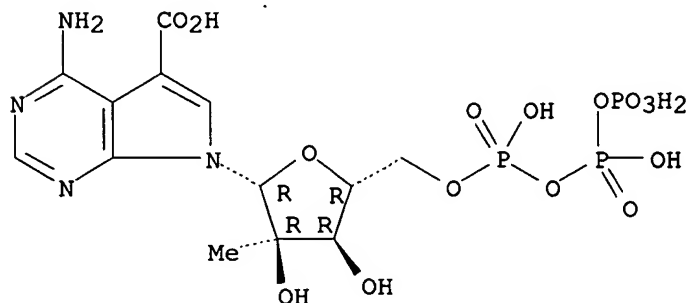
Absolute stereochemistry.



RN 443643-13-8 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-2-C-methyl- $\beta$ -D-ribofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



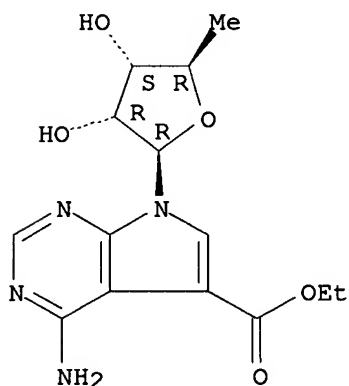
DOCUMENT NUMBER: 137:304253  
 TITLE: QSAR study on adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues using the hansch approach  
 AUTHOR(S): Srikanth, K.; Debnath, Bikash; Jha, Tarun  
 CORPORATE SOURCE: Division of Medicinal and Pharmaceutical Chemistry, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, 700032, India  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(6), 899-902  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB QSAR studies on series of pyrrolo[2,3-d]pyrimidine nucleoside analogs were performed for their adenosine kinase (AK) inhibitory activity using the Hansch approach. Significant correlations were obtained with hydrophobic parameter at position 'X'. Electronic and steric parameters on pyrimidine and pyrrole rings found to play an important role in the ligand-receptor interactions with the active sites of the enzyme. Presence of bulkier groups at 'X' and 'Y' positions seems to protect the title compds. from biodegrdn., as is evident from their pos. sterimol steric parameter B1 at these positions.

IT 144928-02-9  
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (QSAR study on adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogs using the hansch approach)

RN 144928-02-9 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2000:455674 CAPLUS  
 DOCUMENT NUMBER: 133:222942  
 TITLE: Adenosine Kinase Inhibitors. 1. Synthesis, Enzyme Inhibition, and Anti-seizure Activity of 5-Iodotubercidin Analogues  
 AUTHOR(S): Ugarkar, Bheemarao G.; DaRe, Jay M.; Kopcho, Joseph J.; Browne, Clinton E., III; Schanzer, Juergen M.; Wiesner, James B.; Erion, Mark D.  
 CORPORATE SOURCE: Metabasis Therapeutics Inc., San Diego, CA, 92121, USA  
 SOURCE: Journal of Medicinal Chemistry (2000), 43(15), 2883-2893  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal

LANGUAGE: English  
OTHER SOURCE(S): CASREACT 133:222942

AB Adenosine receptor agonists produce a wide variety of therapeutically useful pharmacologies. However, to date they have failed to undergo successful clin. development due to dose-limiting side effects. Adenosine kinase inhibitors (AKIs) represent an alternative strategy, since AKIs may raise local adenosine levels in a more site- and event-specific manner and thereby elicit the desired pharmacol. with a greater therapeutic window. Starting with 5-iodotubercidin ( $IC_{50} = 0.026 \mu M$ ) and 5'-amino-5'-deoxyadenosine ( $IC_{50} = 0.17 \mu M$ ) as lead inhibitors of the isolated human AK, a variety of pyrrolo[2,3-d]pyrimidine nucleoside analogs were designed and prepared by coupling 5-substituted-4-chloropyrrolo[2,3-d]pyrimidine bases with ribose analogs using the sodium salt-mediated glycosylation procedure. 5'-Amino-5'-deoxy analogs of 5-bromo- and 5-iodotubercidins were found to be the most potent AKIs reported to date ( $IC_{50}s < 0.001 \mu M$ ). Several potent AKIs were shown to exhibit anticonvulsant activity in the rat maximal elec. shock (MES) induced seizure assay.

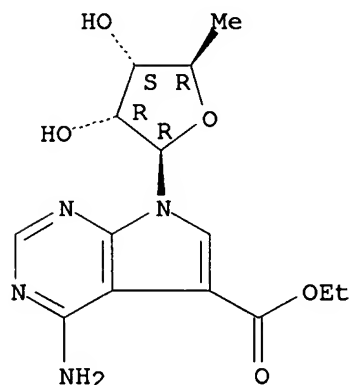
IT 144928-02-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(synthesis, enzyme inhibition, and anti-seizure activity of iodotubercidin analogs)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy- $\beta$ -D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



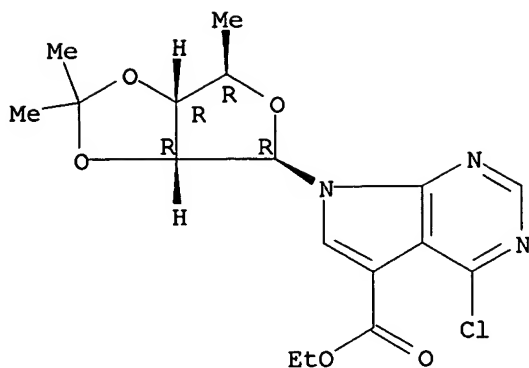
IT 291535-42-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(synthesis, enzyme inhibition, and anti-seizure activity of iodotubercidin analogs)

RN 291535-42-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-[5-deoxy-2,3-O-(1-methylethylidene)- $\beta$ -D-ribofuranosyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:629981 CAPLUS

DOCUMENT NUMBER: 129:260742

TITLE: Preparation of 7-deaza-2'-deoxyguanosine-5'-triphosphate derivatives and their use in DNA sequencing

INVENTOR(S): Fuller, Carl; McDougall, Mark; Kumar, Shiv

PATENT ASSIGNEE(S): Amersham Pharmacia Biotech Inc, USA

SOURCE: Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

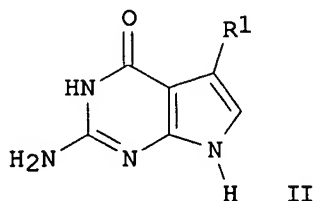
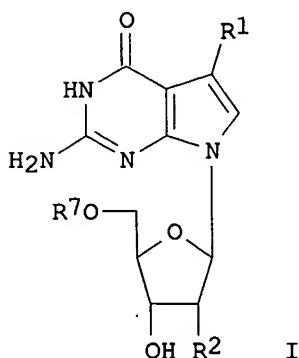
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 866070	A1	19980923	EP 1998-301727	19980309
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
GB 2323357	A1	19980923	GB 1998-5000	19980309
GB 2323357	B2	19990929		
JP 2000119296	A2	20000425	JP 1998-72317	19980320
US 6906185	B1	20050614	US 1998-45732	19980320
PRIORITY APPLN. INFO.:			US 1997-41320P	P 19970320
OTHER SOURCE(S):	MARPAT 129:260742			
GI				



AB The title compds. (I; R1 = C1-10 alkyl optionally substituted with OH, amino, C1-4 alkoxy or halo; R2 = H, OH; R7 = H, mono-, di-, triphosphate

or thiophosphate group; when R1 = Me then R7 ≠ H), useful, e.g., in resolution of compression artifacts in DNA sequencing, were prepared A nucleotide sequence containing I, a DNA acid sequence containing a base II (R1 = C1-10 alkyl, optionally substituted by OH, amino, C1-4 alkoxy or halo), a method for determining the nucleoside base sequence of a DNA mol., a method of elongation of an oligonucleotide sequence, and 7-alkynyl analogs of I are also claimed. For example, esterification of 7-(prop-1-ynyl)-7-deaza-2'-deoxyguanosine and hydrogenation of the resulting 5'-triphosphate ester Et3N-salt with H in the presence of Pd/C gave I (R1 = Pr, R2 = H, R7 = triphosphate group), useful for the title purpose.

IT 213623-53-1P

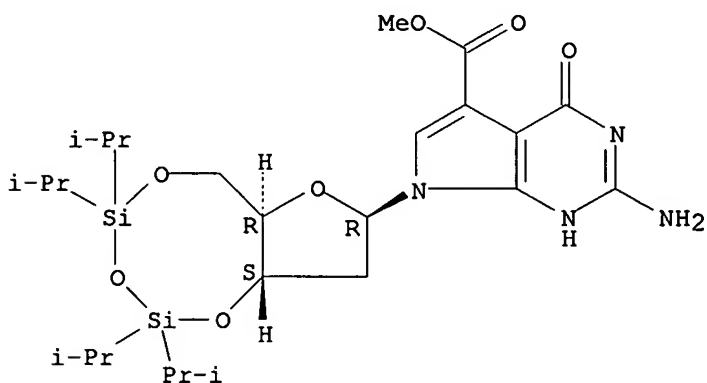
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 7-deaza-2'-deoxyguanosine-5'-triphosphate derivs. and their use in DNA sequencing)

RN 213623-53-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-[2-deoxy-3,5-O-[1,1,3,3-tetrakis(1-methylethyl)-1,3-disiloxanediyl]-β-D-erythro-pentofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:600335 CAPLUS

DOCUMENT NUMBER: 129:316495

TITLE: Facile synthesis of 2'-deoxynucleoside analogs of preQ

AUTHOR(S): Ramzaeva, Natalya; Becher, Georg; Seela, Frank

CORPORATE SOURCE: Laboratorium Organische Bioorganische Chemie, Institut Chemie, Universitaet Osnabrueck, Osnabrueck, D-49069, Germany

SOURCE: Synthesis (1998), (9), 1327-1330

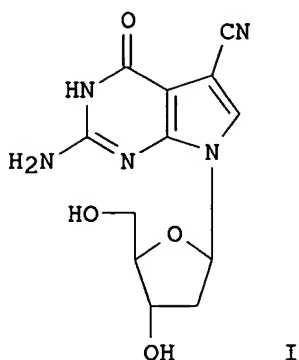
CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The 2'-deoxy derivative of the naturally occurring preQ0 nucleoside I as well as its pyrazolo[3,4-d]pyrimidine analog were synthesized by Cu-mediated cyanation of the corresponding 7-iodo-7-deazaguanine or -8-azaguanine nucleoside. The compds. were converted into the corresponding 7-carboxy 7-carbamoyl derivs.

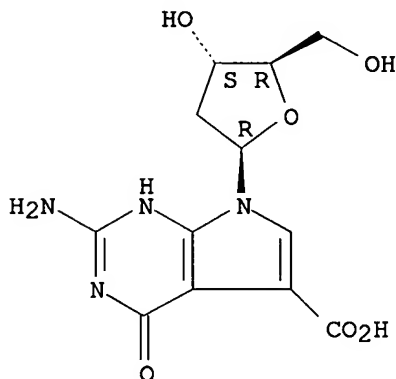
IT **124738-85-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of deoxynucleoside analogs of preQ)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 22 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:102691 CAPLUS

DOCUMENT NUMBER: 124:261553

TITLE: New synthetic routes to 5-substituted pyrrolo(2,3-d)pyrimidines. total synthesis of rigidin and 2'-deoxy-cadeguomycin. synthesis and characterization of novel mesoionic imidazo(1,2-c)pyrimidine-3-ones

AUTHOR(S): Wei, Yuan

CORPORATE SOURCE: Utah State Univ., Logan, UT, USA

SOURCE: (1995) 138 pp. Avail.: Univ. Microfilms Int., Order No. DA9603501

From: Diss. Abstr. Int., B 1995, 56(9), 4894

DOCUMENT TYPE: Dissertation

LANGUAGE: English

AB Unavailable

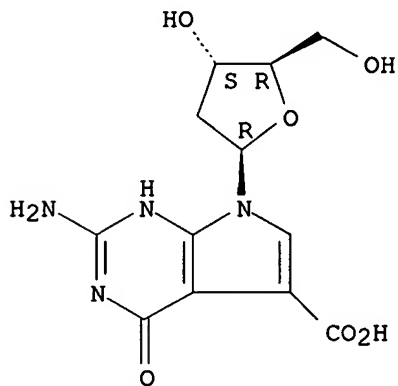
IT **124738-85-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of rigidin and deoxycadeguomycin and preparation and characterization of mesoionic imidazopyrimidinones)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy- $\beta$ -D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 23 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:714164 CAPLUS

DOCUMENT NUMBER: 123:83913

TITLE: A New Synthetic Route to  $\beta$ -2'-Deoxyribosyl-5-Substituted Pyrrolo[2,3-d]pyrimidines. Synthesis of 2'-Deoxycadeguomycin

AUTHOR(S): Edstrom, Eric D.; Wei, Yuan

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Utah State University, Logan, UT, 84322-0300, USA

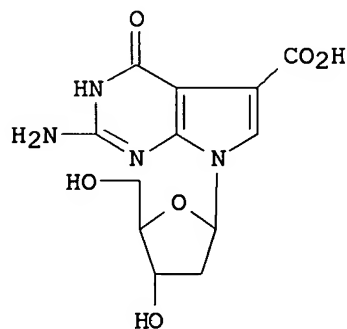
SOURCE: Journal of Organic Chemistry (1995), 60(16), 5069-76  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

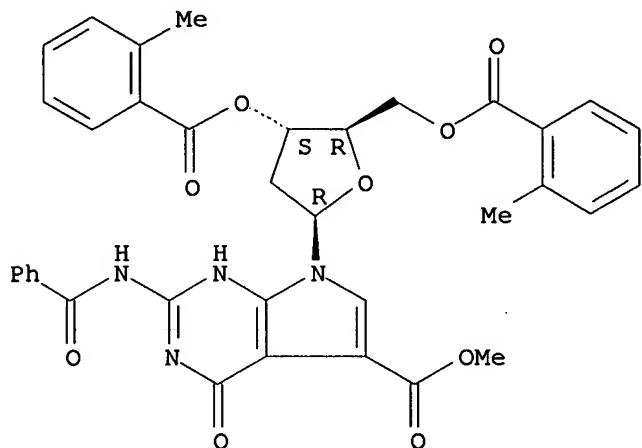


I

AB A new and flexible synthetic route to  $\beta$ -2'-deoxyribosyl-5-substituted pyrrolo[2,3-d]pyrimidines has been developed. Formation of the pyrrole ring is effected by combining sodium N-(4-nitrophenethyl)glycinate with a differently protected 6-chlorouracil derivative generating a substitution adduct. Heating of this material in acetic anhydride affords the 5-(acetyloxy)pyrrolo[2,3-d]pyrimidine 9 in high yield. Base-mediated removal of the pyrrole protecting group gives free pyrrole 10 which is then glycosylated with 1-chloro-2-deoxy-3,5-ditoluoyl- $\alpha$ -D-erythro-pentofuranose using the sodium salt method. The resulting glycosides 15a,b ( $\alpha$ : $\beta$ , 1:4) are readily separated following hydrolysis of the C-5 acetyloxy group. An efficient synthetic route to the pyrrolo[2,3-d]pyrimidine nucleotide analog, deoxycadeguomycin I, is presented. The key transformation involves the conversion of the differentially protected pyrrolo[2,3-d]pyrimidine-2,4-dione base portion into a protected 2-aminopyrrolo[2,3-d]pyrimidin-4-one.

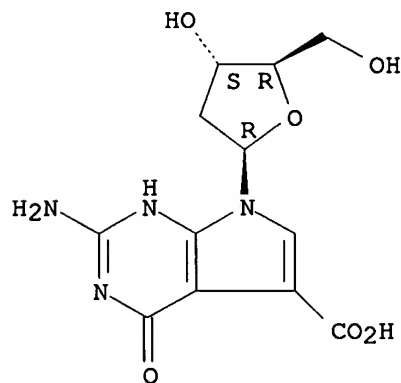
IT **165260-45-7P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of pyrrolopyrimidine deoxyribonucleosides and  
 deoxycadeguomycin)  
 RN 165260-45-7 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(benzoylamino)-7-[2-deoxy-  
 3,5-bis-O-(2-methylbenzoyl)- $\beta$ -D-erythro-pentofuranosyl]-4,7-dihydro-4-  
 oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **124738-85-8P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pyrrolopyrimidine deoxyribonucleosides and  
 deoxycadeguomycin)  
 RN 124738-85-8 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy- $\beta$ -D-  
 erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

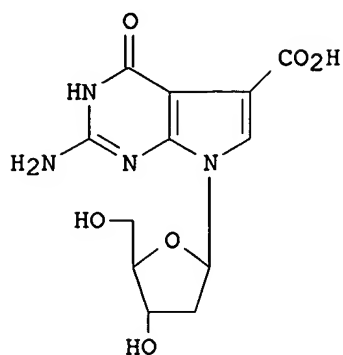
Absolute stereochemistry.



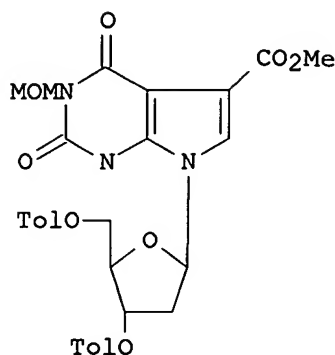
L3 ANSWER 24 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1995:263070 CAPLUS  
 DOCUMENT NUMBER: 122:133655  
 TITLE: Total synthesis of 2'-deoxycadeguomycin, a new  
 pyrrolo[2,3-d]pyrimidine nucleotide analog  
 AUTHOR(S): Edstrom, Eric D.; Wei, Yuan  
 CORPORATE SOURCE: Dep. of Chem. and Biochemistry, Utah State Univ.,  
 Logan, UT, 84322-0300, USA  
 SOURCE: Tetrahedron Letters (1994), 35(48), 8989-90  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal

LANGUAGE:  
OTHER SOURCE(S):  
GI

English  
CASREACT 122:133655



I



II

AB This paper describes an efficient synthetic route to a novel pyrrolo[2,3-d]pyrimidine nucleotide analog, 2'-deoxycadeguomycin I. The key transformation involves the conversion of the differentially protected pyrrolo[2,3-d]pyrimidine-2,4-dione base portion in deoxyribonucleoside II into a protected 2-aminopyrrolo[2,3-d]pyrimidin-4-one.

IT **161087-93-0P**

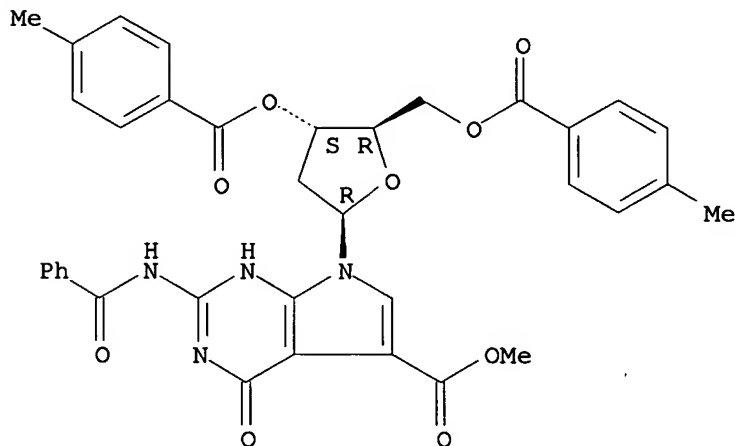
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of deoxycadeguomycin from pyrrolopyrimidinedione deoxyribonucleoside via C-2 amination)

RN 161087-93-0 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(benzoylamino)-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



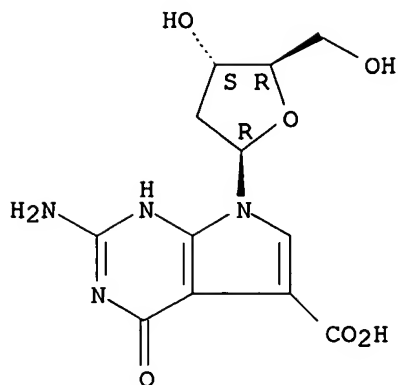
IT **124738-85-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of deoxycadeguomycin from pyrrolopyrimidinedione deoxyribonucleoside via C-2 amination)

RN 124738-85-8 CAPLUS

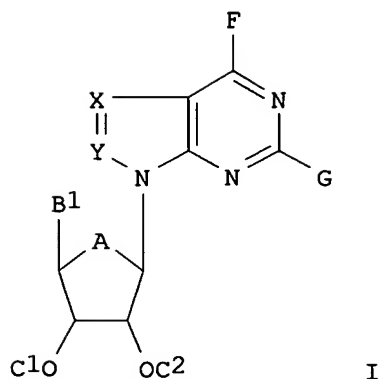
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 25 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1994:621999 CAPLUS  
 DOCUMENT NUMBER: 121:221999  
 TITLE: Preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents  
 INVENTOR(S): Firestein, Gary Steven; Ugarkar, Bheemarao Ganapatrao; Miller, Leonard Paul; Gruber, Harry Edward; Bullough, David Andrew; Erion, Mark David; Castellino, Angelo John  
 PATENT ASSIGNEE(S): Gensia, Inc., USA  
 SOURCE: PCT Int. Appl., 114 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 14  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9417803	A1	19940818	WO 1994-US1340	19940203
W: AT, AU, BB, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9462365	A1	19940829	AU 1994-62365	19940203
EP 682519	A1	19951122	EP 1994-909558	19940203
R: CH, DE, FR, GB, IT, LI				
US 5646128	A	19970708	US 1994-349125	19941201
PRIORITY APPLN. INFO.:			US 1993-14190	A 19930203
			US 1989-408707	B2 19890915
			US 1990-466979	B2 19900118
			US 1991-647117	B2 19910123
			US 1991-812916	B2 19911223
			US 1994-192645	B1 19940203
			WO 1994-US1340	W 19940203
OTHER SOURCE(S):		MARPAT 121:221999		
GI				



AB Novel nucleosides I [A = O, CH<sub>2</sub>, S; B' = (CH<sub>2</sub>)<sub>n</sub>B, alkenyl, alkynyl; B = H, alkyl, alkoxy, NH<sub>2</sub>, alkylamino, etc.; C1, C2 = H, acyl, hydrocarbyloxycarbonyl, or C1C2 = C(:O), α-alkoxyalkylidene; X = CD; D = H, halo, alkyl, cyano, CO<sub>2</sub>H, etc.; Y = N, CE; E = H, halo, alkyl, alkylthio; F = alkyl, aryl, halo, cyano, indolyl, pyrrolidinyl, etc.; G = H, halo, alkyl, alkoxy, alkylamino, alkylthio; n = 1-4], prepared by multistep procedures which are described, selectively inhibit adenosine kinase and are useful in treatment of conditions characterized by an inflammatory response. Such conditions include sepsis, arthritis, autoimmune disease, burns, psoriasis, conjunctivitis, etc. Thus, mice with endotoxemia resulting from injection of *Escherichia coli* lipopolysaccharide showed a dose-dependent increase in survival in response to i.v. injection of the adenosine kinase inhibitor, 4-amino-1-(5-amino-5-deoxy-1-β-D-ribofuranosyl)-3-bromopyrazolo[3,4-d]pyrimidine-HCl; this effect was antagonized by the adenosine receptor antagonist 8-(p-sulphophenyl)theophylline.

IT 144928-02-9P

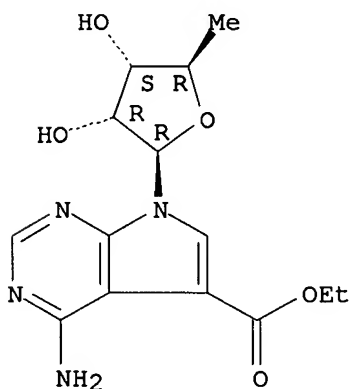
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP. (Preparation); USES (Uses)

(preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 26 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

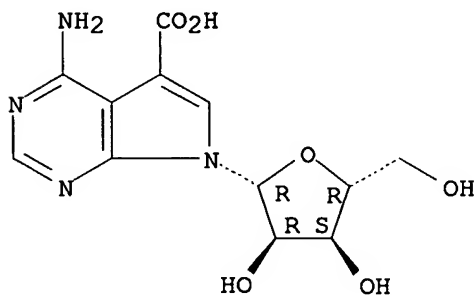
ACCESSION NUMBER: 1994:400251 CAPLUS

DOCUMENT NUMBER: 121:251

TITLE: Relationship between the structure of sangivamycin-derived nucleosides and their effect on leukemic cell growth and on protein kinase A and C activity

AUTHOR(S): Bobek, Miroslav; Bloch, Alexander  
 CORPORATE SOURCE: Dep. Exp. Therap., Roswell Park Cancer Inst., Buffalo, NY, 14263, USA  
 SOURCE: Nucleosides & Nucleotides (1994), 13(1-3), 429-35  
 CODEN: NUNUD5; ISSN: 0732-8311  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The nucleotide antibiotic sangivamycin (4-amino-7-( $\beta$ -D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine-5-carboxamide), is an effective inhibitor of protein kinase A (PKA) and protein kinase C (PKC) but, upon its phosphorylation in intact cells, it gains the ability to affect other targets as well. To retain its selectivity for the protein kinases, a series of nonphosphorylatable sangivamycin derivs. was prepared by replacing the 5'-hydroxyl group with other functions including N3, F, SO<sub>2</sub>NH<sub>2</sub>, NO<sub>2</sub>, and NH<sub>2</sub>,. These derivs. were more potent inhibitors of PKA and PKC than were the phosphorylatable compds., although the latter were more potent inhibitors of leukemic cell growth.  
 IT **18418-00-3**  
 RL: BIOL (Biological study)  
 (antileukemic and protein kinases A and C inhibitory activity of)  
 RN 18418-00-3 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7- $\beta$ -D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 27 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1993:234420 CAPLUS  
 DOCUMENT NUMBER: 118:234420  
 TITLE: Adenosine kinase inhibitors  
 INVENTOR(S): Browne, Clinton E.; Ugarkar, Bheemarao G.; Mullane, Kevin M.; Gruber, Harry E.; Bullough, David A.; Erion, Mark D.; Castellino, Angelo  
 PATENT ASSIGNEE(S): Gensia Pharmaceuticals, Inc., USA  
 SOURCE: Eur. Pat. Appl., 87 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 14  
 PATENT INFORMATION:

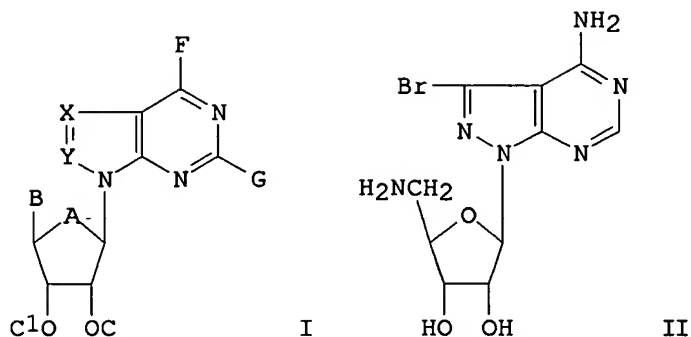
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 496617	A1	19920729	EP 1992-300580	19920123
EP 496617	B1	19991201		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE				
CA 2100863	AA	19920724	CA 1992-2100863	19920121
WO 9212718	A1	19920806	WO 1992-US515	19920121
W: AU, CA, FI, NO				
AU 665184	B2	19951221	AU 1992-13599	19920121
AU 9213599	A1	19920827		
JP 05112595	A2	19930507	JP 1992-10094	19920123
IL 100742	A1	19960618	IL 1992-100742	19920123
AT 187175	E	19991215	AT 1992-300580	19920123
NO 9302628	A	19930923	NO 1993-2628	19930721

NO 180418  
NO 180418  
US 5646128  
PRIORITY APPLN. INFO.:

B 19970106  
C 19970416  
A 19970708

US 1994-349125 19941201  
US 1991-647117 A 19910123  
US 1991-812916 A 19911223  
US 1989-408707 B2 19890915  
US 1990-466979 B2 19900118  
WO 1992-US515 W 19920121  
US 1993-14190 B2 19930203  
US 1994-192645 B1 19940203

OTHER SOURCE(S): MARPAT 118:234420  
GI



AB Nucleoside analogs I [A = O, CH<sub>2</sub>, S; B = (un)substituted C1-4 alkyl; C, Cl = H, protective group(s); X = (un)substituted CH; Y = N, (un)substituted CH; F = alkyl, aryl, aralkyl, halogen, (un)substituted NH<sub>2</sub>, substituted OH or SH, cyano, cyanoalkyl; G = H, halogen, alkyl, alkoxy, alkylamino, alkylthio] were prepared. Thus, the analog II was prepared from the pyrimidinone via the azide. II has an adenosine kinase-inhibiting ED<sub>50</sub> of <10 nM and was effective in improving post-ischemic functional recovery in isolated guinea pig heart and in preclin. angina models.

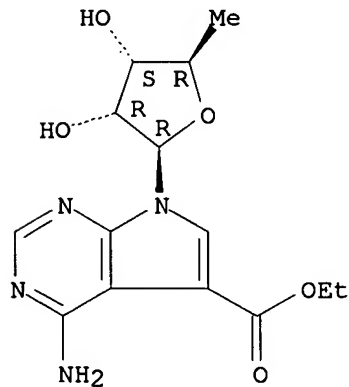
IT 144928-02-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



TITLE: Structure-activity relationships for cadeguomycin analogs

AUTHOR(S): Kim, Sun Hee; Okazaki, Kimitake; Okabe, Takayoshi; Nishimura, Toshio; Kondo, Tadao; Tanaka, Nobuo; Suzuki, Hideo

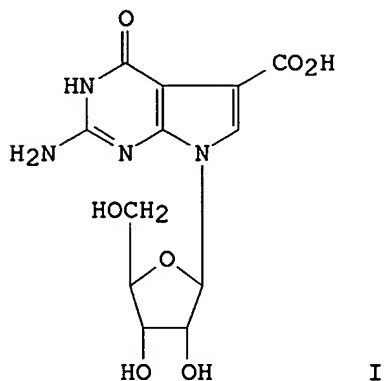
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Antibiotics (1991), 44(6), 659-64  
CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



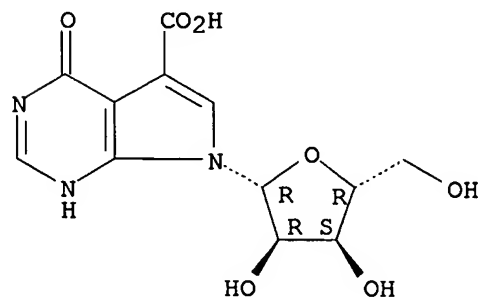
AB The relationship between the antitumor activity and the chemical structure of cadeguomycin (CDM, I) was studied with 6 analogs of CDM. Both activities of CDM, enhancing the incorporation of [3H]thymidine in K562 cells and potentiating the cytotoxicity of cytosine arabinoside for K562 cells, were significantly augmented by the replacement of the 7-carboxyl group with cyano (CDM-CN) or formyl (CDM-CHO), but they were not changed by the replacement with Me. The activities were almost completely diminished by the replacement of ribose with arabinose, but the simultaneous replacement of carboxyl and ribose with formyl and arabinose showed higher activities than those of CDM. The replacement of 7-carboxy-7-deazaguanine with 7-carboxy-7-deazainosine markedly weakened the activity. CDM-CN and CDM-CHO at 0.2 µg/mL significantly potentiated the activity of cytosine arabinoside against MOLT-3 cells but CDM at 1 µg/mL did not. Thus, the ribose and guanine moieties in the CDM mol. are very important for its activity. Also replacing the carboxyl group at the C-7 position with cyano or formyl group is a useful way to strengthen the CDM activity. These compds. would effectively potentiate cytosine arabinoside against various kinds of tumor cells which CDM could not do.

IT 28070-52-2 81645-08-1 81645-08-1D,  
Cadeguomycin, analogs 104846-27-7  
RL: BIOL (Biological study)  
(ara-C cytotoxicity potentiation by, structure in relation to)

RN 28070-52-2 CAPLUS

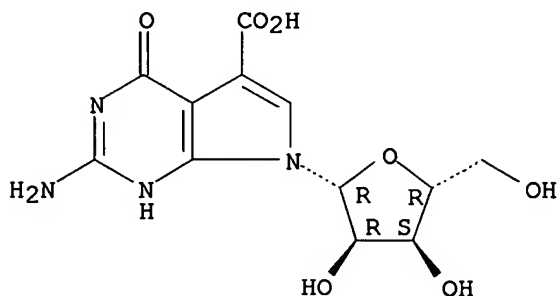
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



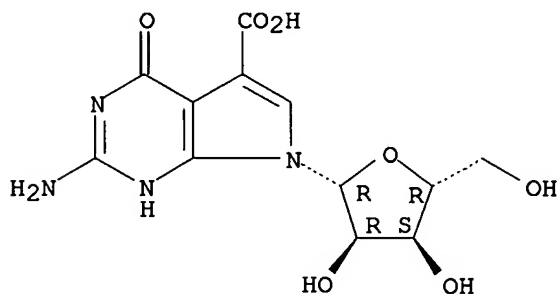
RN 81645-08-1 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-  
β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



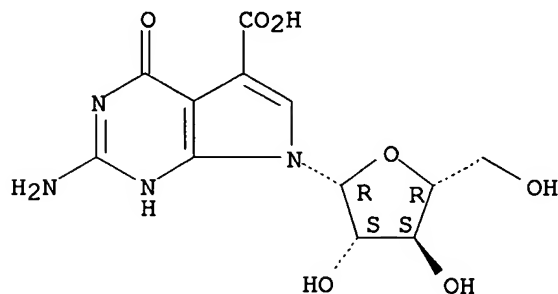
RN 81645-08-1 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-  
β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



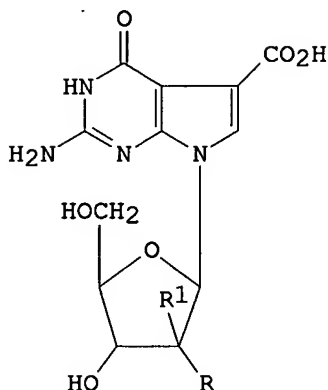
RN 104846-27-7 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-  
arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

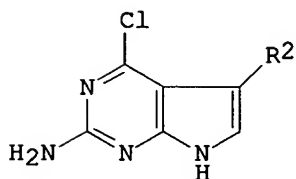


L3 ANSWER 29 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1990:217442 CAPLUS  
DOCUMENT NUMBER: 112:217442  
TITLE: Total and stereospecific synthesis of cadeguomycin,  
2'-deoxycadequomycin, ara-cadequomycin, and certain  
related nucleosides  
AUTHOR(S): Ramasamy, Kandasamy; Joshi, Ramachandra V.; Robins,  
Roland K.; Revankar, Ganapathi R.  
CORPORATE SOURCE: Dep. Med. Chem., ICN Nucl. Acid Res. Inst., Costa  
Mesa, CA, 92626, USA  
SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1972-1999)

DOCUMENT TYPE:  
LANGUAGE:  
OTHER SOURCE(S):  
GI



I



II

AB A total and stereospecific synthesis of the title cadeguomycins I (R = OH, R1 = H; R = R1 = H; R = H, R1 = OH) was accomplished from the novel aglycons II (R2 = cyano, CO2Me). Ring annulation of 2,6-diaminopyrimidin-4(3H)-one with Me chloro(formyl)acetate in the presence of NaOAc provided a mixture of two products from which the desired Me 2-amino-3,4-dihydro-4-oxo-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylate was separated and converted into II. Several 2-amino-4,5-disubstituted pyrrolo[2,3-d]pyrimidine nucleosides were also prepared

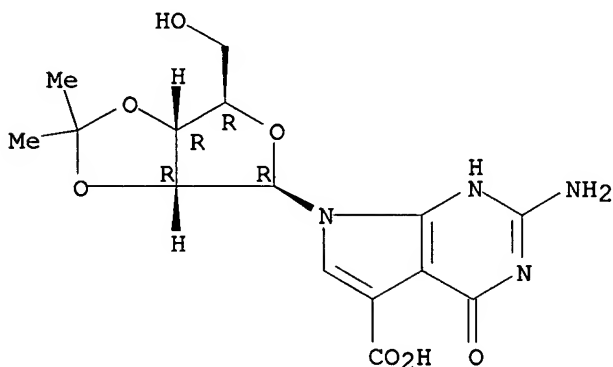
IT 127070-81-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and conversion of, to cadeguomycin)

RN 127070-81-9 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-7-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



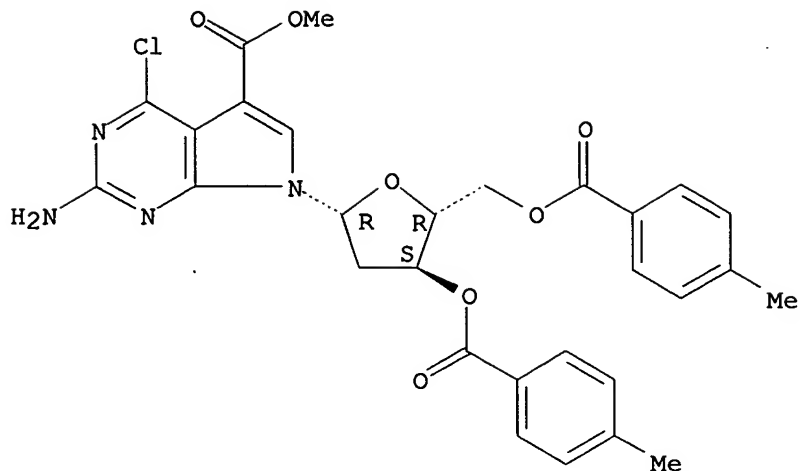
IT 124738-86-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and conversion of, to deoxycadeguomycin)

RN 124738-86-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



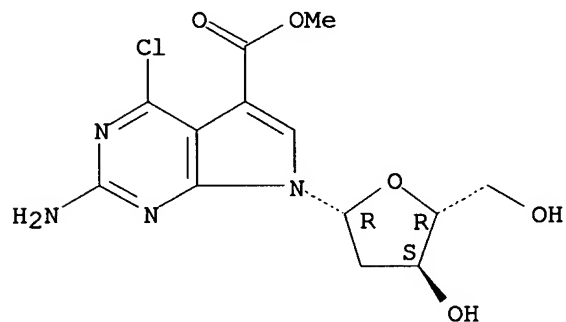
IT 127047-55-6P 127047-56-7P 127047-57-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 127047-55-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-(2-deoxy-β-D-erythro-pentofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

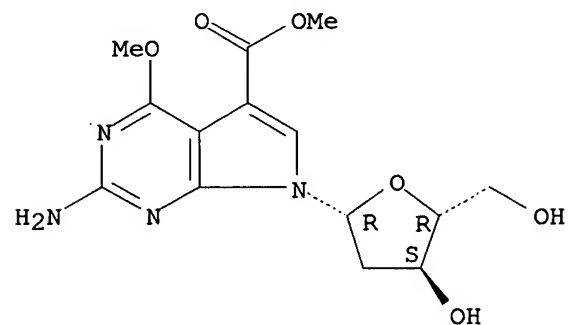
Absolute stereochemistry.



RN 127047-56-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

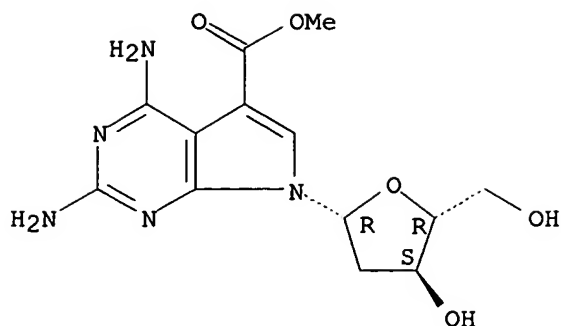
Absolute stereochemistry.



RN 127047-57-8 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2,4-diamino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 81645-08-1P, Cadeguomycin 104846-27-7P, ara-Cadeguomycin

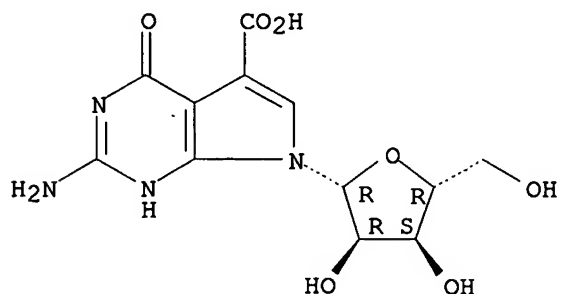
124738-85-8P, 2'-Deoxycadeguomycin

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(total stereospecific synthesis of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

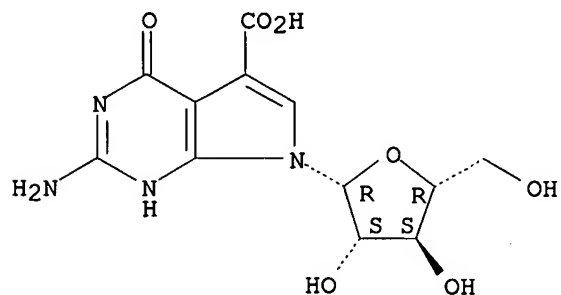
Absolute stereochemistry.



RN 104846-27-7 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

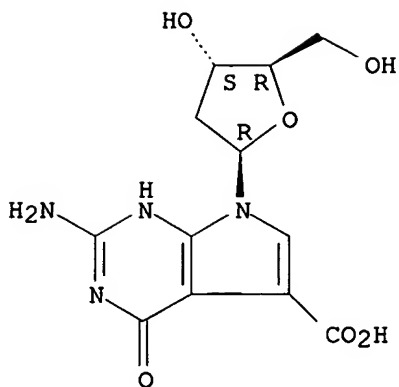
Absolute stereochemistry.



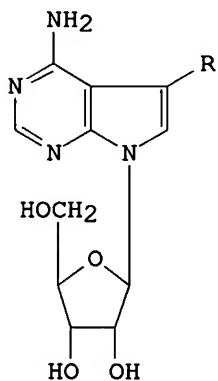
RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 30 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1990:155489 CAPLUS  
 DOCUMENT NUMBER: 112:155489  
 TITLE: The isolation and structure of modified bioactive nucleosides from *Jaspis johnstoni*  
 AUTHOR(S): Zabriskie, T. Mark; Ireland, Chris M.  
 CORPORATE SOURCE: Dep. Med. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA  
 SOURCE: Journal of Natural Products (1989), 52(6), 1353-6  
 CODEN: JNPRDF; ISSN: 0163-3864  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

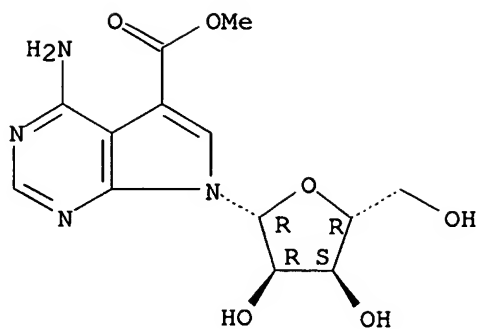


I, R=CN  
 II, R=CO<sub>2</sub>Me

AB Two cytotoxic pyrrolo[2,3-d]pyrimidine nucleosides, toyocamycin (I) and 5-(methoxycarbonyl)tubercidin (II) were isolated from the Fijan sponge *J. johnstoni*. The structures were solved primarily by <sup>13</sup>C-NMR and mass spectral methods and confirmed by comparison to reported values in the literature. Small amts. of the corresponding aglycons were also isolated.

IT **18440-68-1**  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of sponge)  
 RN 18440-68-1 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 31 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:56513 CAPLUS

DOCUMENT NUMBER: 112:56513

TITLE: Total and stereospecific synthesis of 2'-deoxycadeguomycin

AUTHOR(S): Ramasamy, Kandasamy; Robins, Roland K.; Revankar, Ganapathi R.

CORPORATE SOURCE: Dep. Med. Chem., ICN Nucl. Acid Res. Inst., Costa Mesa, CA, 92626, USA

SOURCE: Journal of the Chemical Society, Chemical Communications (1989), (9), 560-2  
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:56513

AB An efficient and stereospecific synthesis of 2'-deoxycadeguomycin from both 7-deazapurine derivs. 2-amino-4-chloropyrrolo[2,3-d]pyrimidine-5-carbonitrile and Me 2-amino-4-chloropyrrolo[2,3-d]pyrimidine-5-carboxylate has been accomplished.

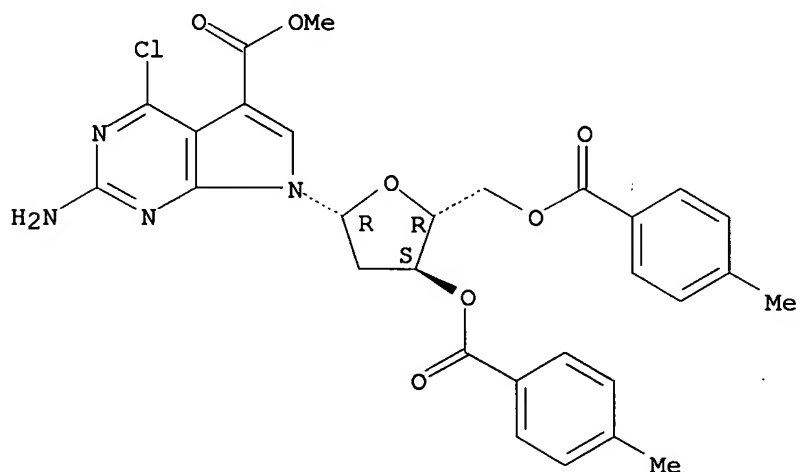
IT **124738-86-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and conversion of, to deoxycadeguomycin)

RN 124738-86-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



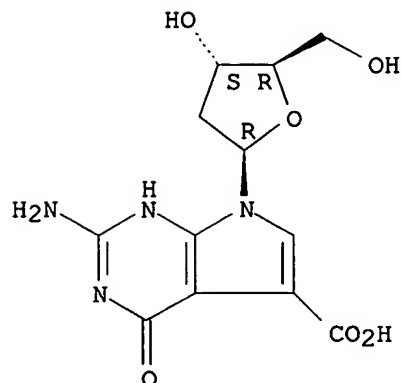
IT **124738-85-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 32 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:147191 CAPLUS

DOCUMENT NUMBER: 110:147191

TITLE: Comparative studies of the inhibitory properties of antibiotics on human immunodeficiency virus and avian myeloblastosis virus reverse transcriptases and cellular DNA polymerases

AUTHOR(S): Take, Yukinori; Inouye, Yoshio; Nakamura, Shoshiro; Allaudeen, H. S.; Kubo, Akinori

CORPORATE SOURCE: Sch. Med., Hiroshima Univ., Hiroshima, 734, Japan

SOURCE: Journal of Antibiotics (1989), 42(1), 107-115

CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The inhibition of human immunodeficiency virus (HIV) reverse transcriptase by certain antibiotics and related compds. was studied in comparison with that of avian myeloblastosis virus (AMV) reverse transcriptase and cellular DNA polymerases  $\alpha$  and  $\beta$ . In general, compds. that inhibited HIV reverse transcriptase also inhibited AMV reverse transcriptase. For example, 10  $\mu\text{g/mL}$  of the isoquinoline quinones used in this study inhibited approx. 80% of the activity of reverse transcriptases of HIV and AMV, but did not inhibit the activity of DNA polymerases  $\alpha$  and  $\beta$  even at 50  $\mu\text{g/mL}$ . AMV enzyme was more sensitive than HIV enzyme to colistin, enduracidins A and B, janiemycin, glyasperin A, and thielavins A and B. The streptonigrin alkyl esters, however, inhibited HIV reverse transcriptase only. Sakyomicin A, luzopeptins, ellagic acid and suramine inhibited the activities of reverse transcriptases and cellular DNA polymerases. Structure-activity relations are discussed.

IT 81645-08-1, Cadeguomycin

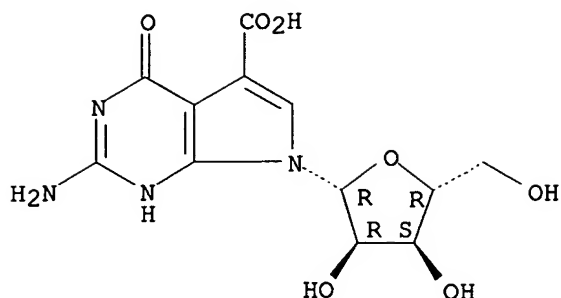
RL: BIOL (Biological study)

(DNA polymerase and human immunodeficiency virus and avian myeloblastosis virus reverse transcriptase inhibition by, structure in relation to)

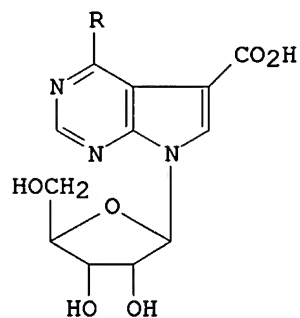
RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

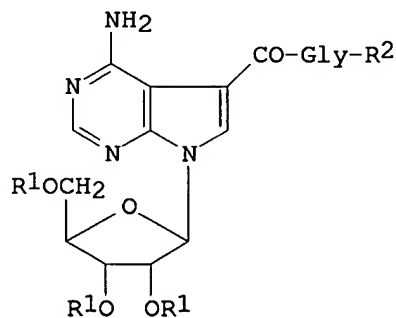
Absolute stereochemistry.



L3 ANSWER 33 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1988:590805 CAPLUS  
 DOCUMENT NUMBER: 109:190805  
 TITLE: Nucleoside peptides. IX. Synthesis of peptide derivatives of sangivamycic acid and deaminosangivamycic acid  
 AUTHOR(S): Ramasamy, Kandasamy; Robins, Roland K.; Revankar, Ganapathi R.  
 CORPORATE SOURCE: Dep. Med. Chem., Nucleic Acid Res. Inst., Costa Mesa, CA, 92626, USA  
 SOURCE: Tetrahedron (1988), 44(4), 1023-34  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 109:190805  
 GI



I

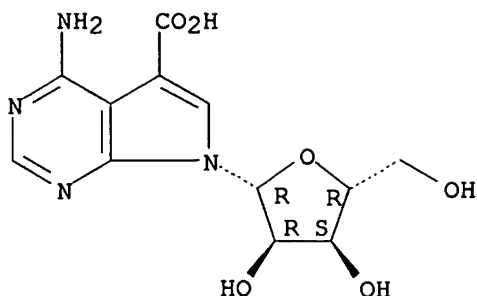


IV

AB Amino acid and peptide conjugates of sangivamycic acid (I, R = NH<sub>2</sub>) (II) and deaminosangivamycic acid (I, R = OH) (III) were prepared in which the peptide linkage is on the carboxylic group of the aglycon moiety. The formation of these conjugates was accomplished via coupling of I or II with protected amino acids or peptides mediated by Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>N:C:NEt.HCl/1-hydroxybenzotriazole. Thus, II was condensed with H-Gly-OEt and then O-acetylated with Ac<sub>2</sub>O in DMF/pyridine to give nucleoside peptide IV (R<sub>1</sub> = Ac, R<sub>2</sub> = OEt), which was treated with NH<sub>3</sub>/MeOH to give IV (R<sub>1</sub> = H, R<sub>2</sub> = NH<sub>2</sub>).

IT **18418-00-3P**, Sangivamycic acid **28070-52-2P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and condensation with amino acids and peptides)  
 RN 18418-00-3 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

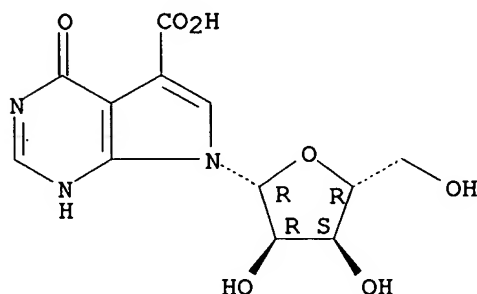
Absolute stereochemistry.



RN 28070-52-2 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



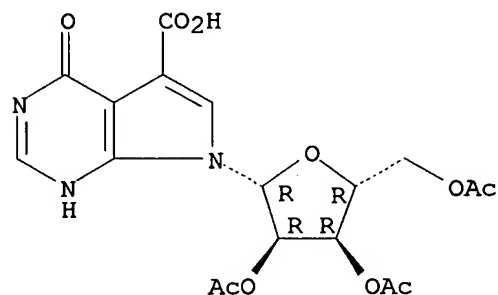
IT 117175-66-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation with arginine derivative)

RN 117175-66-3 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



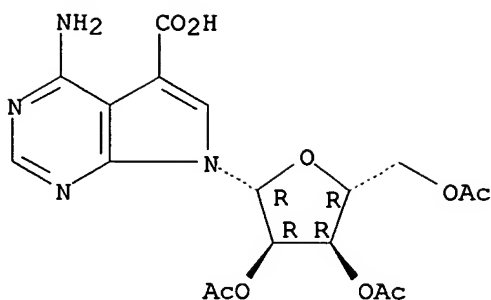
IT 117175-46-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and condensation with glycine Et ester)

RN 117175-46-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 34 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:68455 CAPLUS

DOCUMENT NUMBER: 108:68455

TITLE: Effects of cadeguomycin on cytotoxicity of cytosine arabinoside and other pyrimidine nucleoside analogs; a comparative study

AUTHOR(S): Kim, Sun Hee; Okabe, Takayoshi; Tanaka, Nobuo; Suzuki, Hideo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Antibiotics (1987), 40(12), 1776-7

CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cadeguomycin at 1 µg/mL did not affect the growth of K562 human myelogenous leukemia cells alone, but it potentiated the cytotoxicity of cytosine arabinoside 56.4-fold and that of 5-fluorodeoxycytidine 10.2-fold. The effects of cadeguomycin on the cytotoxicity of other pyrimidine nucleoside and base analogs were less notable. The decrease of deoxycytidine monophosphate deaminase activity in K562 cells may be related to the neoplasm inhibitor-potentiating effect.

IT **81645-08-1**, Cadeguomycin

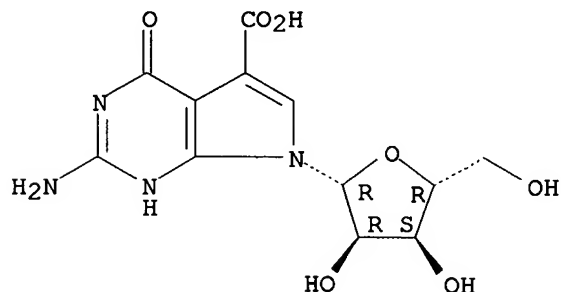
RL: BIOL (Biological study)

(neoplasm inhibition by pyrimidine nucleosides increase by, in humans)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 35 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:176807 CAPLUS

DOCUMENT NUMBER: 106:176807

TITLE: 5-De-carboxy-5-formylcadeguomycin analogs

INVENTOR(S): Okamoto, Kaoru; Goto, Toshio; Tanaka, Nobuo

PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

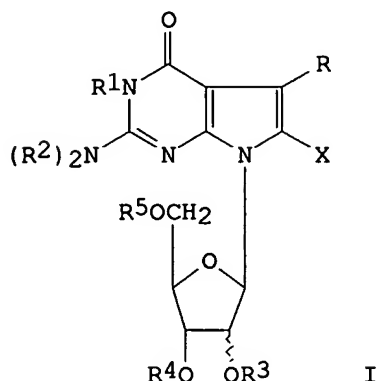
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61229897	A2	19861014	JP 1985-73256	19850405
JP 05060478	B4	19930902		

PRIORITY APPLN. INFO.:  
GI

JP 1985-73256 19850405



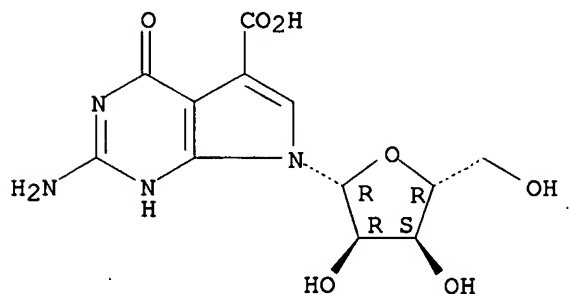
AB The title compound (I; R = CHO; R1-R5 = X = H), useful as an anticancer agent, was prepared. Thus, hydrogenolysis of D-ribo-I (R = CH2OH, R1 = CH2OMe, R2 = R5 = Ac, R3R4 = Me2C, X = Br) in aqueous MeOH containing AcOK over Pd/C, oxidation of the resulting D-ribo-I (X = H) in MeCN with MnO2 for 1/2 h followed by ammonolysis and hydrolysis with aqueous CF3CO2H at 70° for 1 h gave D-ribo-I (R = CHO, R1-R5 = X = H). This at 10 µg/mL in vitro inhibited by 50% the growth of mouse lymphatic leukemia L5178Y cells and in vitro enhanced the incorporation of 3H-thymidine into human leukemia K562 cells. Tablets and capsules containing the title compds. were prepared.

IT **81645-08-1**, Cadeguomycin  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(esterification of, with methanol)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 36 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:131367 CAPLUS

DOCUMENT NUMBER: 106:131367

TITLE: Potentiation of cytotoxicity of 1-β-D-arabinofuranosylcytosine for K562 Human leukemic cells by cadeguomycin

AUTHOR(S): Suzuki, Hideo; Kim, Sun Hee; Tahara, Makoto; Okazaki, Kimitake; Okabe, Takayoshi; Wu, Rong Tsun; Tanaka, Nobuo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Cancer Research (1987), 47(3), 713-17

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The treatment of K562 human myeloblastic leukemia cells and YAC-1 murine lymphoma cells with cadeguomycin [81645-08-1] at concns.  $>0.6 \mu\text{M}$  significantly enhanced the cytotoxicity of 1- $\beta$ -D-arabinofuranosylcytosine (ara-C) [147-94-4]. The degree of potentiation depended upon the antibiotic concentration. The treatment with  $75 \mu\text{M}$  cadeguomycin for 18 h increased cellular uptake of  $[3\text{H}]\text{ara-C}$  into K562 cells and formation of ara-C nucleotides, as well as incorporation into nucleic acids. The level of the ara-C diphosphate plus the ara-C triphosphate was approx. 10 times higher in the cadeguomycin-treated cells than in the untreated cells by 30 min of incubation with  $[3\text{H}]\text{ara-C}$ . The exts. of  $15 \mu\text{M}$  cadeguomycin-treated K562 cells showed increased activity of formation of ara-C nucleotides, resulting in 4- to 5-fold higher formation of the di- and triphosphates of ara-C than the control cell exts. Cadeguomycin did not significantly change the level of ribonucleotide and deoxyribonucleotide pool in K562 cells. The mechanism of potentiation of ara-C by cadeguomycin is discussed.

IT 81645-08-1, Cadeguomycin

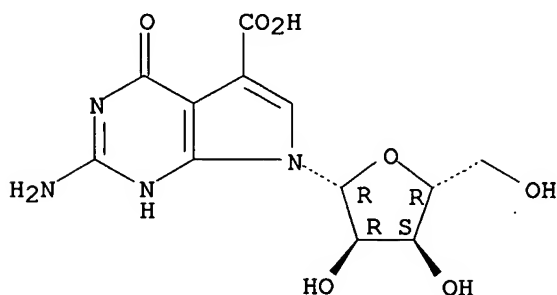
RL: BIOL (Biological study)

(cytotoxicity of arabinofuranosylcytosine potentiation by)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 37 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:43284 CAPLUS

DOCUMENT NUMBER: 106:43284

TITLE: Studies on substances effective against antitumor drug-resistant tumor cells

AUTHOR(S): Suzuki, Hideo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan

SOURCE: Medicina Philosophica (1986), 5(8), 646-8

CODEN: MDPHDG; ISSN: 0286-2190

DOCUMENT TYPE: Journal; General Review

LANGUAGE: Japanese

AB A review, with 6 refs., on the mechanism of acquired tolerance of tumor cells to chemotherapeutic agents and the effectiveness of cadeguomycin [81645-08-1] and lactoquinomycin A [100100-36-5] against the tolerance when they were obtained with other neoplasm inhibitors.

IT 81645-08-1

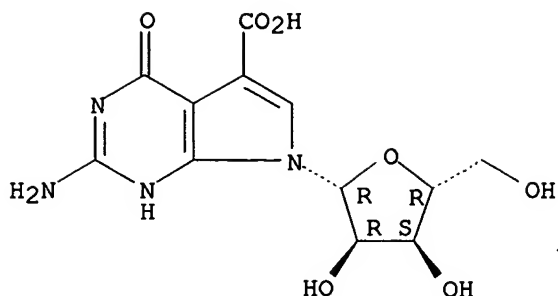
RL: BIOL (Biological study)

(drug resistance to neoplasm inhibitors response to)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 38 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:618445 CAPLUS

DOCUMENT NUMBER: 105:218445

TITLE: Potentiation of arabinosylcytosine-induced erythroid differentiation of human leukemia K562 cells by cadeguomycin

AUTHOR(S): Wu, R. T.; Chen, S. C.; Tien, W. C.; Tanaka, N.

CORPORATE SOURCE: Grad. Program Microbiol. Immunol., Natl. Yang-Ming Med. Coll., Taipei, Taiwan

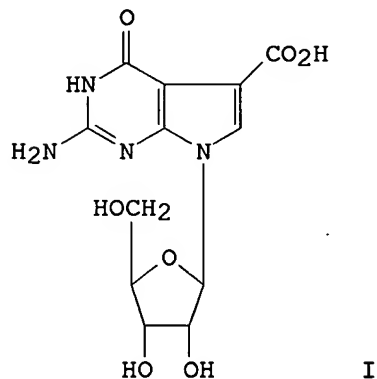
SOURCE: Recent Adv. Chemother., Proc. Int. Congr. Chemother., 14th (1985), Volume Anticancer Sect. 1, 201-2. Editor(s): Ishigami, Joji. Univ. Tokyo Press: Tokyo, Japan.

CODEN: 55GNAX

DOCUMENT TYPE: Conference

LANGUAGE: English

GI



AB Cadeguomycin (I) [81645-08-1] enhanced the induction of erythroid differentiation in human myelogenous leukemic cells K562 treated with low concns. of ara-C [147-94-4]. In the presence of a low concentration (0.1 µg/mL) of ara-C, I markedly increased the amount of Hb synthesized, up to 20-fold even at a concentration of 1 µg I/mL. The 2 main forms of Hb synthesized by K562 cells in the presence of I and ara-C were Hb Gower-1 [56592-05-3] and Hb Portland [54846-99-0]. After induction of erythroid differentiation by cadeguomycin and ara C, K562 cells lost their clonogenic properties in soft agar medium and tumorigenicity in nude mice.

IT 81645-08-1

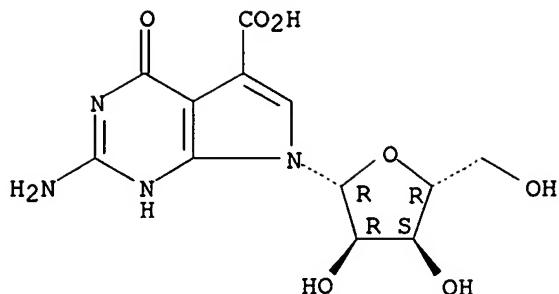
RL: BIOL (Biological study)

(arabinosylcytosine-induced erythroid differentiation of human leukemia cell potentiation by)

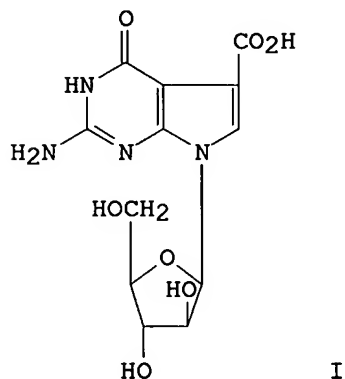
RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

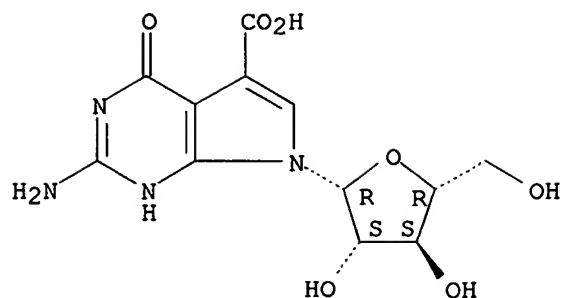


L3 ANSWER 39 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1986:572961 CAPLUS  
 DOCUMENT NUMBER: 105:172961  
 TITLE: Synthesis of ara-cadeguomycin. 2-Amino-3,4-dihydro-4-oxo-7-(β-D-arabinofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid  
 AUTHOR(S): Okamoto, Kaoru; Kondo, Tadao; Goto, Toshio  
 CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan  
 SOURCE: Bulletin of the Chemical Society of Japan (1986), 59(6), 1915-19  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:172961  
 GI



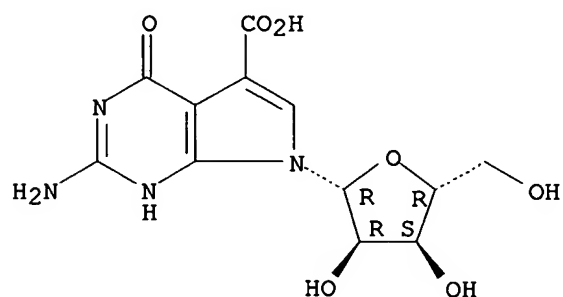
AB The title nucleoside (I), an analog of cadeguomycin, was prepared via glycosylation of 3-methoxymethyl-5-methyl-2-methylthio-7H-pyrrolo[2,3-d]pyrimidin-4(3H)-one with 2,3,5-tri-O-benzyl-D-arabinofuranosyl chloride.  
 IT **104846-27-7P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 104846-27-7 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

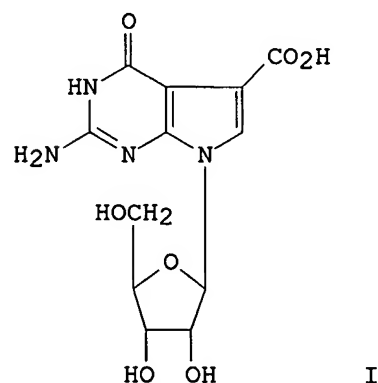


IT **81645-08-1DP**, analog  
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of)  
 RN 81645-08-1 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-  
 β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 40 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1986:497859 CAPLUS  
 DOCUMENT NUMBER: 105:97859  
 TITLE: A total synthesis of cadeguomycin, a nucleoside  
 antibiotic produced by *Streptomyces hygroscopicus*  
 Kondo, Tadao; Okamoto, Kaoru; Yamamoto, Manabu; Goto,  
 Toshio; Tanaka, Nobuo  
 AUTHOR(S):  
 CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan  
 SOURCE: Tetrahedron (1986), 42(1), 199-205  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:97859  
 GI



AB The nucleoside antibiotic cadeguomycin (I) was prepared from

3,4-3-methoxymethyl-5-methyl-2-methylthio-7-(2,3-O-isopropylidene-5-O-triphenylmethyl- $\beta$ -D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidin-4-one, which was effectively prepared by glycosylation of 3,4-dihydro-3-methoxymethyl-5-methyl-2-methylthio-7H-pyrrolo-[2,3-d]pyrimidin-4-one with 2,3-O-isopropylidene-5-O-triphenylmethyl- $\beta$ -D-ribofuranosyl chloride.

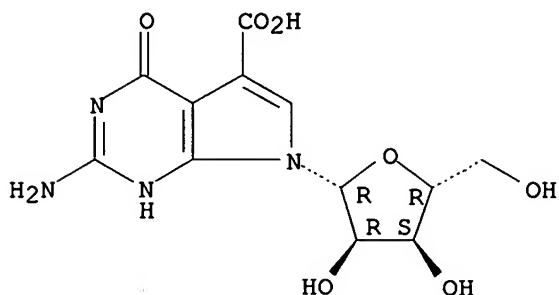
IT **81645-08-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 41 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:28534 CAPLUS

DOCUMENT NUMBER: 104:28534

TITLE: Enhancement of pyrimidine nucleoside uptake into K562 and YAC-1 cells by cadeguomycin

AUTHOR(S): Wu, Rong Tsun; Okabe, Takayoshi; Kim, Sun Hee; Suzuki, Hideo; Tanaka, Nobuo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Antibiotics (1985), 38(11), 1588-95

CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

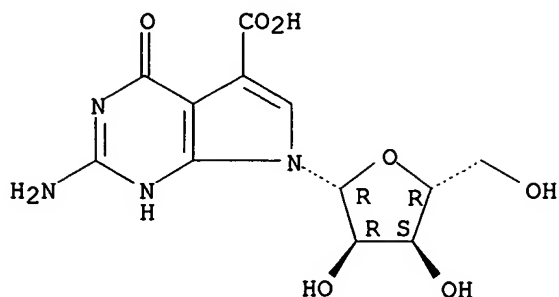
AB Cadequomycin [**81645-08-1**] markedly stimulated the uptake of thymidine [50-89-5], deoxycytidine [951-77-9], and uridine [58-96-8] into the acid-insol. fraction of K562 human leukemic cells, but did not affect adenosine [58-61-7] incorporation. The enhancement of pyrimidine nucleoside uptake was 6-17-fold over the control. Aspartate incorporation into nucleic acid was not significantly blocked by the antibiotic, suggesting that the stimulation of pyrimidine nucleoside incorporation is not due to the inhibition of de novo pyrimidine nucleotide synthesis. Net DNA and RNA syntheses, observed by [<sup>32</sup>P]phosphate uptake were not affected by cadequomycin. The enzymic activity of thymidine kinase [9002-06-6], deoxycytidine kinase [9039-45-6], and uridine kinase [9026-39-5] was higher in cadequomycin-treated cells than in untreated cells, suggesting that the enhancement of pyrimidine nucleoside uptake occurs in the phosphorylation process. The stimulatory activity of cadequomycin of thymidine uptake was reversed by guanosine [118-00-3] and deoxyguanosine [961-07-9], but not by adenosine and deoxyadenosine, suggesting that intracellular metabolism and/or action of cadequomycin is related to that of guanosine and deoxyguanosine. The stimulation of pyrimidine nucleoside incorporation by cadequomycin was also found with YAC-1 cells, but not with the other cell lines. The enhancement effect of the antibiotic seems to be not directly related to its cytotoxicity.

IT **81645-08-1**

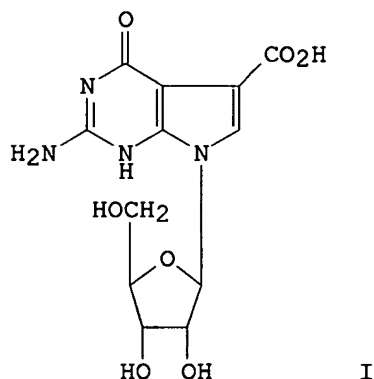
RL: BIOL (Biological study)  
(pyrimidine nucleoside uptake by leukemia cells of human enhancement by, kinase activity in relation to)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)



L3 ANSWER 42 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:416522 CAPLUS  
 DOCUMENT NUMBER: 103:16522  
 TITLE: Biological activity of cadeguomycin. Inhibition of tumor growth and metastasis, immunostimulation, and potentiation of 1-β-D-arabinofuranosylcytosine  
 AUTHOR(S): Yuan, Bao Ding; Wu, Rong Tsun; Sato, Isao; Okabe, Takayoshi; Suzuki, Hideo; Nishimura, Toshio; Tanaka, Nobuo  
 CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan  
 SOURCE: Journal of Antibiotics (1985), 38(5), 642-8  
 CODEN: JANTAJ; ISSN: 0021-8820  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



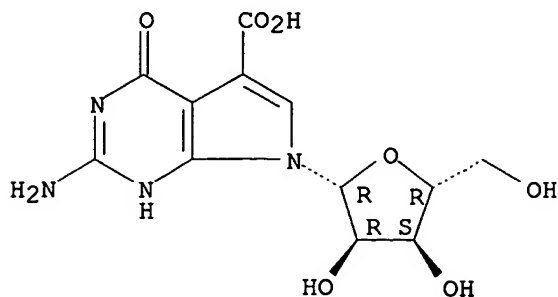
AB Cadeguomycin (I) [81645-08-1] retarded the growth of s.c. solid IMC carcinoma and the pulmonary metastasis of Lewis lung carcinoma in mice. The antibiotic enhanced phagocytic activity of murine peritoneal macrophages and interleukin-1 production by P388D1 cells. Delayed-type hypersensitivity was stimulated and interferon was induced by the drug. The results suggest that I inhibits tumor growth and metastasis in association with modification of the immune system. The cytotoxicity of 1-β-D-arabinosylcytosine [147-94-4] to K562 and YAC-1 cells was markedly enhanced by I in culture. The combined administration of arabinosylcytosine and I displayed potentiation of the inhibition of growth of i.p. implanted P388 leukemia and metastasis of s.c. implanted P388 leukemia to the regional lymph nodes. I showed low toxicity in mice.

IT 81645-08-1  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (antineoplastic activity of, metastasis inhibition and immunostimulation and arabinofuranosylcytosine cytotoxicity potentiation in relation to)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 43 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:531021 CAPLUS

DOCUMENT NUMBER: 101:131021

TITLE: Fast atom bombardment combined with tandem mass spectrometry for the determination of nucleosides  
AUTHOR(S): Crow, Frank W.; Tomer, Kenneth B.; Gross, Michael L.; McCloskey, James A.; Bergstrom, Donald E.

CORPORATE SOURCE: Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588, USA

SOURCE: Analytical Biochemistry (1984), 139(1), 243-62

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The pos. and neg. ion fast atom bombardment (FAB) mass spectra and fast atom bombardment collisionally activated decomposition (CAD) spectra of a series of nucleosides and 2 dinucleotides are reported. The nucleosides studied are substituted forms of guanosine, adenosine, nebularine, tubercidin, uridine, and related pyrimidines. The FAB and CAD data both contain similar information. The CAD spectra provide some structural information not found in the FAB mass spectra. Tandem mass spectrometry also allows emphasis to be put on weak fragments which are either not observed in the FAB mass spectrum or are lost in the matrix ion signals.

IT 18440-68-1

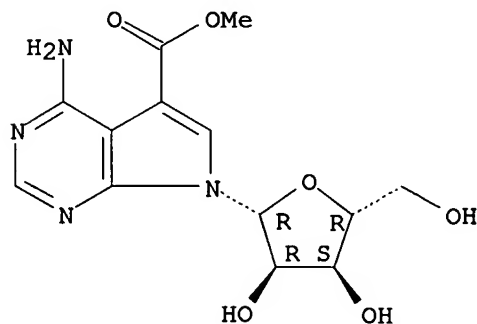
RL: PRP (Properties)

(fast-atom-bombardment mass spectra and pos.-atom-bombardment tandem mass spectra of)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7- $\beta$ -D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 44 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:103800 CAPLUS

DOCUMENT NUMBER: 100:103800

TITLE: Pyrrolopyrimidine nucleosides. 19. A total synthesis of the nucleoside antibiotic cadeguomycin

AUTHOR(S):

[2-amino-7-( $\beta$ -D-ribofuranosyl)pyrrolo[2,3-d]pyrimidin-4-one-5-carboxylic acid]  
Beylin, Vladimir G.; Kawasaki, Andrew M.; Cheng, Chin Shu; Townsend, Leroy B.

CORPORATE SOURCE:

Dep. Med. Chem., Coll. Pharm., Ann Arbor, MI, 48109, USA

SOURCE:

Tetrahedron Letters (1983), 24(44), 4793-6  
CODEN: TELEAY; ISSN: 0040-4039

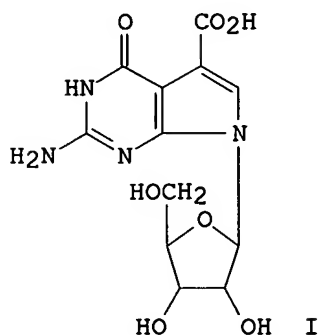
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



AB A total synthesis of the title nucleoside I was accomplished and confirmed the previous structural assignment for the antibiotic cadeguomycin.

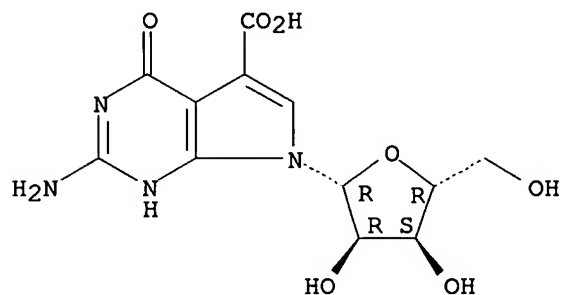
IT **88970-16-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 88970-16-5 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



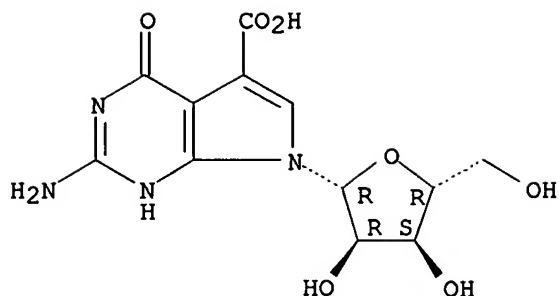
IT **81645-08-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 45 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:61483 CAPLUS

DOCUMENT NUMBER: 100:61483

TITLE: Recent studies on mechanism of action of three antitumor antibiotics

AUTHOR(S): Tanaka, Nobuo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan

SOURCE: Trends Antibiot. Res.: Genet., Biosynth., Actions New

Subst., Proc. Int. Conf. (1982), 79-88. Editor(s):

Umezawa, Hamao; Demain, Arnold L.; Hata, Toju. Jpn.

Antibiot. Res. Assoc.: Tokyo, Japan.

CODEN: 50VJAT

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The mechanism of action of 3 antitumor antibiotics (neothramycin [67298-49-1], 2-crotonyloxymethyl-4,5,6-trihydroxycyclohex-2-enone (COTC) [62532-49-4], and cadeguomycin [81645-08-1]) is discussed. Neothramycin binds to the 2-amino group of a guanine base of DNA. COTC is a multifunctional agent affecting many SH-containing substances, DNA polymerase  $\alpha$ , and mitotic processes. The mechanism of action of cadeguomycin remains to be clarified, although it seems to involve pyrimidine metabolism

IT 81645-08-1

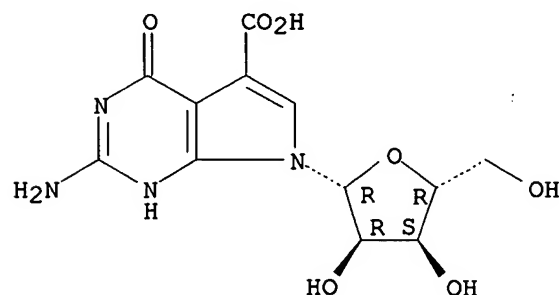
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(neoplasm-inhibiting activity of, mechanism of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 46 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:7038 CAPLUS

DOCUMENT NUMBER: 100:7038

TITLE: Synthesis of cadeguomycin (7-deazaguanosine-7-carboxylic acid)

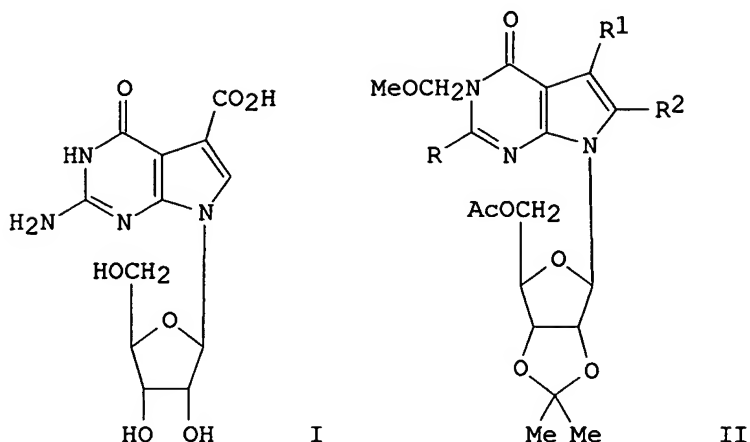
AUTHOR(S): Kondo, Tadao; Goto, Toshio

CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan

SOURCE: Tetrahedron Letters (1983), 24(34), 3647-50

DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: TELEAY; ISSN: 0040-4039  
Journal  
English



AB Cadeguomycin (I) was prepared from deazaguanosine II (R = Ac<sub>2</sub>N, R<sub>1</sub> = Me, R<sub>2</sub> = Br) in 5 steps via  $\alpha$ -hydroxylation, oxidation and debromination.

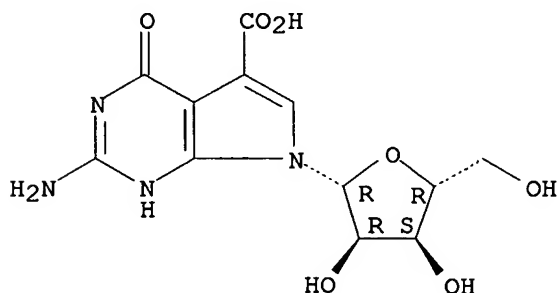
IT **81645-08-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7- $\beta$ -D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 47 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:612871 CAPLUS

DOCUMENT NUMBER: 99:212871

TITLE: Nucleosides and nucleotides. 47. Conversion of tubercidin to toyocamycin: some properties of tubercidin derivatives

AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru

CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

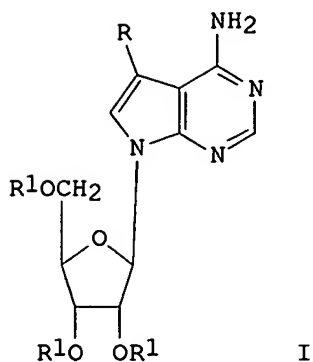
SOURCE: Nucleosides & Nucleotides (1983), 2(2), 113-25

CODEN: NUNUD5; ISSN: 0732-8311

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Tubercidin (I; R = R1 = H) was converted into toyocamycin (I; R = cyano, R1 = H) in 6 steps via the following sequence of intermediates: I [R, R1 given; (morpholinomethyl), H; (morpholinomethyl), Ac; (1-oxidomorpholinomethyl), Ac; CHO, Ac; and CH:NOH, H]. The NMR and CD spectra of 5- and 6-substituted tubercidins show that 6-substituted tubercidins have the syn-conformation in solution

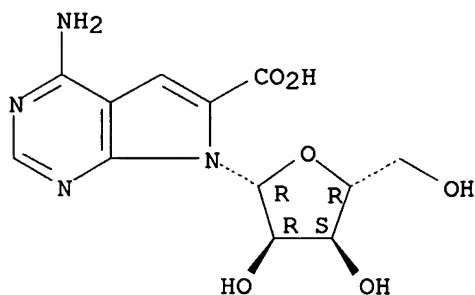
IT 77049-87-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(NMR and CD of)

RN 77049-87-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 48 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:538171 CAPLUS

DOCUMENT NUMBER: 99:138171

TITLE: Cadeguomycin

PATENT ASSIGNEE(S): Microbiochemical Research Foundation, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

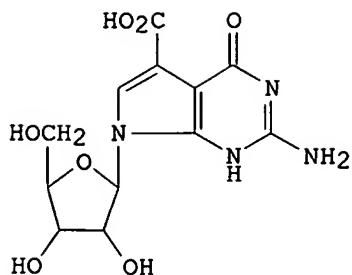
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58092693	A2	19830602	JP 1981-189158	19811127
JP 01039437	B4	19890821		
PRIORITY APPLN. INFO.: GI			JP 1981-189158	19811127



I

AB Cadeguomycin (I) [81645-08-1] was produced by Streptomyces IM791T, freshly isolated from soil and related to S. hygroscopicus ISP5578. Thus, the strain was cultured in a medium containing 2% oatmeal and 0.1% yeast extract at 27° for 114 h. The filtrate (90 L) was treated with Amberlite XAD-8 and the eluate fractionated to give 20.8 mg I. I had no antibacterial activity at 100 µg/mL, but enhanced the activity of ara-C [147-94-4] against human leukemia K562 cells.

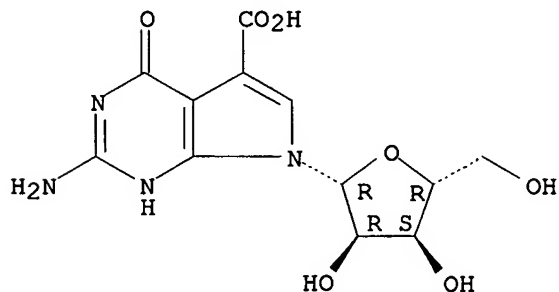
IT 81645-08-1

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (from Streptomyces)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 49 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:437106 CAPLUS

DOCUMENT NUMBER: 99:37106

TITLE: Antibiotic AB-116

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

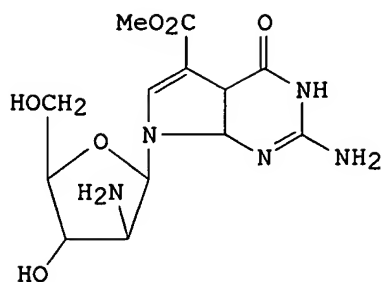
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58032893	A2	19830225	JP 1981-129121	19810817
JP 01053677	B4	19891115		
PRIORITY APPLN. INFO.:			JP 1981-129121	19810817

GI



I

AB Antibiotic AB-116 (I) [86330-89-4] was produced by fermentation with *Actinoplanes kanagawaensis* 232-4 followed by chromatog. Thus, precultured *A. kanagawaensis* 232-4 (Bikoken 6094, FERM P-6094) was cultured on 100 L broth containing glucose 1.5, soybean powder 1.5, NaCl 0.3, and CaCO<sub>3</sub> 0.1% for 120 h at 30° under 50 L/min aeration. The broth filtrate was chromatographed over Diaion Hp-20, Amberlite IRC-50 (H type), Sephadex G-10, and Sephadex LH20 to give 500 mg I. UV and IR spectra of I are shown. I inhibited gram-neg. bacteria.

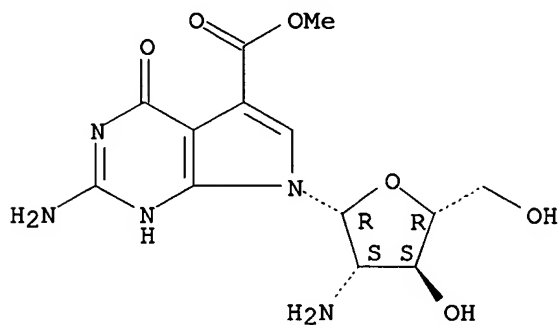
IT 84873-16-5

RL: BIOL (Biological study)  
(from *Actinoplanes kanagawaensis*)

RN 84873-16-5 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-amino-2-deoxy-β-D-arabinofuranosyl)-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 50 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:125711 CAPLUS

DOCUMENT NUMBER: 98:125711

TITLE: Kanagawamicin, a new aminonucleoside analog antibiotic from *Actinoplanes kanagawaensis*

AUTHOR(S): Naruto, Shunsuke; Uno, Hitoshi; Tanaka, Akira; Kotani, Hirotsada; Takase, Yoshiyuki

CORPORATE SOURCE: Res. Lab., Dainippon Pharm. Co., Ltd., Suita, 564, Japan

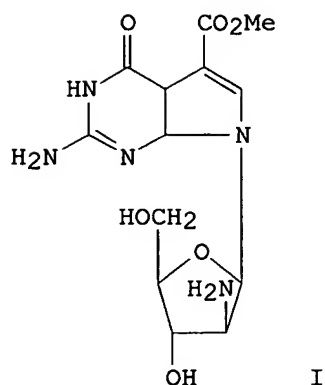
SOURCE: Heterocycles (1983), 20(1), 27-32

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



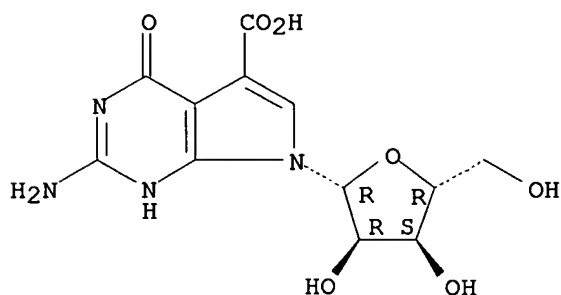
AB The structure of kanagawamicin (I), a new aminonucleoside from *Actinoplanes kanagawaensis*, was deduced from physicochem. data obtained using the natural compound and its acetates.

IT **81645-08-1**  
 RL: PRP (Properties)  
 (NMR spectra of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

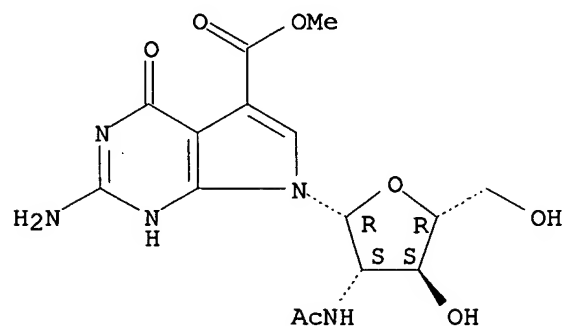


IT **84873-19-8P 84933-22-2P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 84873-19-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-[2-(acetylamino)-2-deoxy-β-D-arabinofuranosyl]-2-amino-4,7-dihydro-4-oxo-, methyl ester (9CI)  
 (CA INDEX NAME)

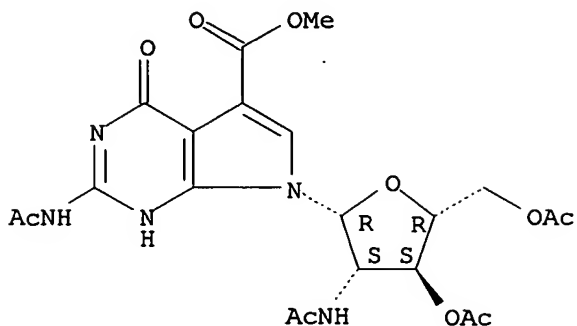
Absolute stereochemistry.



RN 84933-22-2 CAPLUS

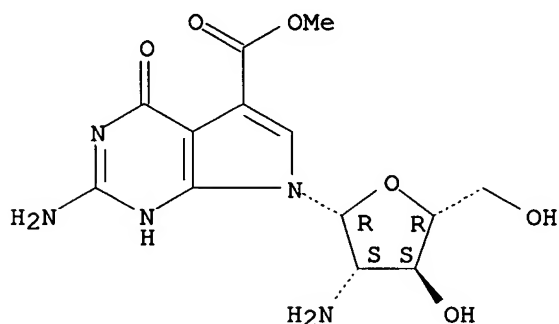
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(acetylamino)-7-[3,5-di-O-acetyl-2-(acetylamino)-2-deoxy-β-D-arabinofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

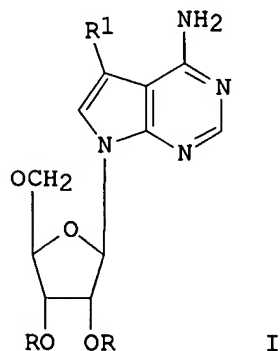


IT **84873-16-5**  
RL: PROC (Process)  
(structural elucidation of)  
RN 84873-16-5 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-amino-2-deoxy- $\beta$ -D-arabinofuranosyl)-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 51 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1983:72659 CAPLUS  
DOCUMENT NUMBER: 98:72659  
TITLE: Nucleosides and nucleotides. 41. Thiocyanation of tubercidin and its derivation to 6-propyl- and 6-cyano derivatives  
AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru  
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan  
SOURCE: Nucleosides & Nucleotides (1982), 1(2), 191-203  
CODEN: NUNUD5; ISSN: 0732-8311  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



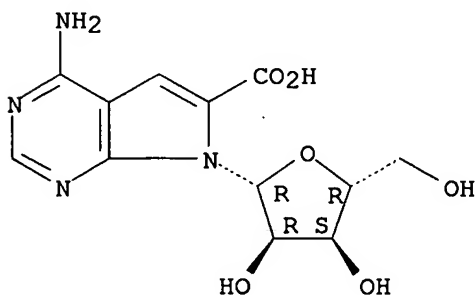
AB Acetylating tubercidin (I; R = R1 = H) with Ac2O-pyridine gave I (R = Ac, R1 = H), which on thiocyanation with KSCN and Cl gave I (R = Ac, R1 = thiocyanato) (II). II was converted into I (R = Ac, R1 = MeS), I (R = H, R1 = MeSO2) (III) and 6-propyltubercidin. III was converted into 6-cyanotubercidin. Also prepared were 6,5'-O-cyclotubercidins.

IT **77049-87-7P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 77049-87-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 52 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:11156 CAPLUS

DOCUMENT NUMBER: 98:11156

TITLE: Pyrrolopyrimidine lethality in relation to ribonucleic acid synthesis in Sarcoma 180 cells in vitro

AUTHOR(S): Ritch, Paul S.; Helmsworth, Marilyn

CORPORATE SOURCE: Dep. Med., Med. Coll. Wisconsin, Milwaukee, WI, 53226, USA

SOURCE: Biochemical Pharmacology (1982), 31(16), 2686-8  
 CODEN: BCPA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

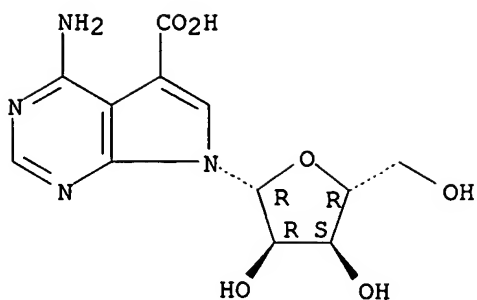
AB Following 1 h exposure of sarcoma 180 cells to sangivamycin (I) [18417-89-5], sangivamycin-amidoxime (II) [22242-94-0], and sangivamycin-amidine (III) [18418-00-3] (all 5 + 10-6M), comparable degrees of cell killing were produced. Relatively few cells were killed following exposure to thiosangivamycin (IV) [22242-90-6]. The relative cytotoxicities were I > II > IV, but for RNA synthesis inhibition by the drugs, the order of potency was reversed. At 1 h following exposure to I, IV, and II, total RNA synthesis was inhibited 24, 73, and 57%, resp. Neither adenosine [58-61-7] nor 2'-deoxycoformycin [53910-25-1] (5 + 10-6M) sep. had any effect on cell survival in response to I, but in combination, they protected against the cytotoxic effects of I.

IT **18418-00-3**  
 RL: PRP (Properties)  
 (cytotoxicity of, RNA formation inhibition in)

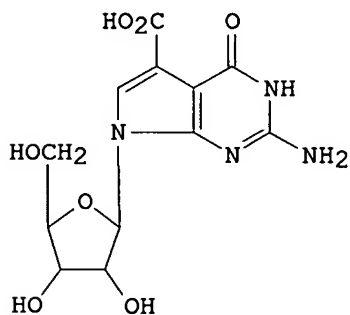
RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 53 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1982:404557 CAPLUS  
 DOCUMENT NUMBER: 97:4557  
 TITLE: Cadeguomycin, a novel nucleoside analog antibiotic.  
 I. The producing organism, production and isolation  
 of cadeguomycin  
 AUTHOR(S): Tanaka, Nobuo; Wu, Rong Tsun; Okabe, Takayoshi;  
 Yamashita, Hide; Shimazu, Akira; Nishimura, Toshio  
 CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan  
 SOURCE: Journal of Antibiotics (1982), 35(3), 272-8  
 CODEN: JANTAJ; ISSN: 0021-8820  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

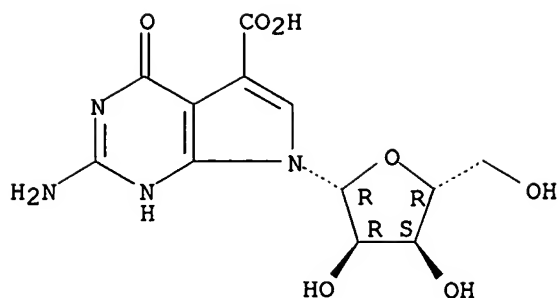
AB An actinomycete strain IM7912T was found to produce cadeguomycin (I) [81645-08-1], a new nucleoside analog antibiotic, together with tubercidin [69-33-0]. Morphol., cultural and physiol. studies showed that the organism belongs to the species *Streptomyces hygroscopicus*. Comparison with *S. hygroscopicus* ISP 5578 revealed that both strains possess similar characteristics except for production of yellow or brownish yellow soluble pigment in some media. I was isolated from the culture filtrate, separated from tubercidin, and purified.

IT 81645-08-1  
 RL: BAC (Biological activity or effector, except adverse); BIOL  
 (Biological study)  
 (tumor inhibitor, from *Streptomyces hygroscopicus*)

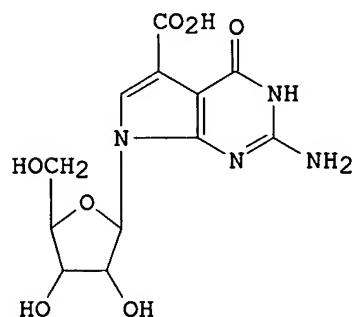
RN 81645-08-1 CAPLUS

CN 1H-Pyrazolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



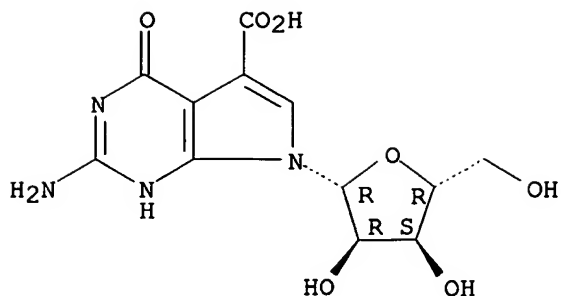
L3 ANSWER 54 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1982:196238 CAPLUS  
 DOCUMENT NUMBER: 96:196238  
 TITLE: Cadeguomycin, a novel nucleoside analog antibiotic.  
 II. Improved purification, physicochemical properties  
 and structure assignment  
 AUTHOR(S): Wu, Rong Tsun; Okabe, Takayoshi; Namikoshi, Michio;  
 Okuda, Shigenobu; Nishimura, Toshio; Tanaka, Nobuo  
 CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan  
 SOURCE: Journal of Antibiotics (1982), 35(3), 279-84  
 CODEN: JANTAJ; ISSN: 0021-8820  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



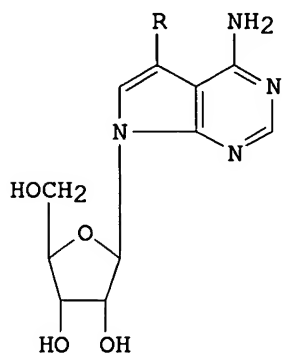
I

AB cadeguomycin (I) [81645-08-1] was isolated from the culture  
 filtrate of *Streptomyces hygroscopicus* by column chromatog. on Amberlite  
 XAD-8 or Amberlite IRA-400, followed by recycling preparative  
 high-pressure column chromatog. The purified antibiotic had a mol.  
 formula of C<sub>12</sub>H<sub>14</sub>O<sub>7</sub>N<sub>4</sub> and a m.p. of 231-9°. The structure of I was  
 determined by NMR spectroscopic anal. as 7-carboxy-7-deazaguanosine.  
 IT 81645-08-1  
 RL: BIOL (Biological study)  
 (antibiotic, from *Streptomyces hygroscopicus*)  
 RN 81645-08-1 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-  
 β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 55 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1981:175411 CAPLUS  
 DOCUMENT NUMBER: 94:175411  
 TITLE: Introduction of substituents to the 7(8)-position of  
 7-deazaadenosine (tubercidin): conversion to  
 toyocamycin  
 AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru  
 CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan  
 SOURCE: Nucleic Acids Symposium Series (1980), 8, s21-s24  
 CODEN: NACSD8; ISSN: 0261-3166  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

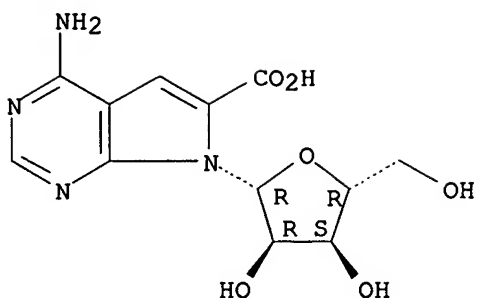


I, R=H  
 II, R=cyano

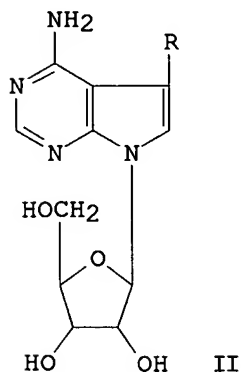
AB Treatment of 2',3',5'-tri-O-acetyl-7-deazaadenosine with ClSCN gave the  
 7-thiocyanato derivative, which was converted to 7-methylthio and  
 7-methylsulfone derivs. The thio-Claisen rearrangement and  
 desulfurization of 7-allylthio derivative gave 8-propyl-7-deazaadenosine. The  
 7-methylsulfone derivative gave the 8-cyano compound by treatment with NaCN.  
 Nitration of triacetyltubercidin gave a mixture of the 7- and 8-nitro  
 derivs. The Mannich reaction of tubercidin (I) gave the  
 7-morpholinomethyl derivative which was converted to the Me, formyl,  
 hydroxymethyl, or cyano derivs. in good yield. The conversion of I to  
 toyocamycin (II) was thus accomplished. Some phys. (spectral and  
 conformational) and biol. (tuberculostatic) properties of these  
 substituted tubercidins are presented.

IT **77049-87-7P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 77049-87-7 CAPLUS  
 CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-  
 ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 56 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1981:157180 CAPLUS  
 DOCUMENT NUMBER: 94:157180  
 TITLE: Pyrrolo[2,3-d]pyrimidine nucleoside antibiotic  
 analogs. Synthesis via organopalladium intermediates  
 derived from 5-mercuritubercidin  
 AUTHOR(S): Bergstrom, Donald E.; Brattesani, Alan J.; Ogawa, Mark  
 K.; Schweickert, Michael J.  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA  
 SOURCE: Journal of Organic Chemistry (1981), 46(7), 1423-31  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB C-5-substituted pyrrolo[2,3-d]pyrimidine nucleosides were synthesized via reactions of 5-mercuritubercidin (I). Pd-catalyzed carbonylation of I in MeOH gave nucleoside II (R = CO<sub>2</sub>Me), which was converted to sangivamycin by reaction with NH<sub>3</sub>. Vinyl analogs (II, R = CH:CHCONH<sub>2</sub>, CH:CHCN) of sangivamycin and toyocamycin were obtained by a Heck organopalladium olefin coupling reaction. II (R = CH:CHCO<sub>2</sub>Me), obtained from I and CH<sub>2</sub>:CHCO<sub>2</sub>Me in the presence of Li<sub>2</sub>PdCl<sub>4</sub>, was converted to (E)-5-(2-bromoethenyl)tubercidin by hydrolysis with base followed by treatment with bromosuccinimide in DMF. The coupling reactions with ethylene, 3-chloro-1-butene, and styrene were also investigated. Ethylene, I and 0.1 M Li<sub>2</sub>PdCl<sub>4</sub> in MeOH lead to II (R = CHMeOMe) and in water to tubercidin (II, R = H), and II (R = CHMeOH). Tubercidin resulted from acid-catalyzed retro-aldol fragmentation. Iodination of I gave II (R = iodo).

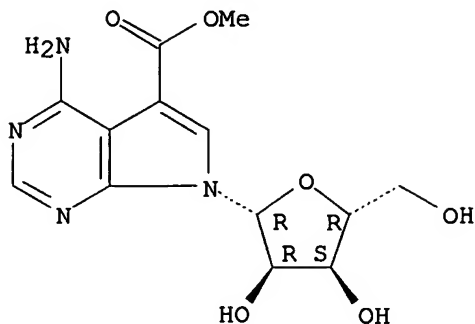
IT 18440-68-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with ammonia)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 57 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:10332 CAPLUS

DOCUMENT NUMBER: 80:10332

TITLE: 5-Hydroxymethyltubercidin. Synthesis, biological activity, and role in pyrrolopyrimidine biosynthesis  
AUTHOR(S): Uematsu, Takayoshi; Suhadolnik, Robert J.  
CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Tokyo, Japan  
SOURCE: Journal of Medicinal Chemistry (1973), 16(12), 1405  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 5-Hydroxymethyltubercidin (I) [49558-38-5] gave 50% growth inhibition of leukemia L-1210 cells at 4 .tim. 10<sup>-7</sup> M while toyocamycin (II) [606-58-6] gave 50% inhibition at 4 .tim. 10<sup>-8</sup> M. II inhibits both L-1210 and bacterial (Escherichia coli and Mycobacterium phlei) cells while I is selective, only inhibiting L-1210 cells. When I labeled with 3H was added to cultures of Streptomyces rimosus at the time of II production, there was an uptake of I but no conversion to II. I was prepared from tubercidin-5-carboxylic acid (III) [18418-00-3] [prepared from sangivamycin (IV) [18417-89-5]] by conversion to the methyl ester (V), then to the 2',3'-O-isopropylidene derivative and LiAlH<sub>4</sub> reduction (method A) or by first protecting the 6-amino group of V with Ph<sub>3</sub>CCl (method B).

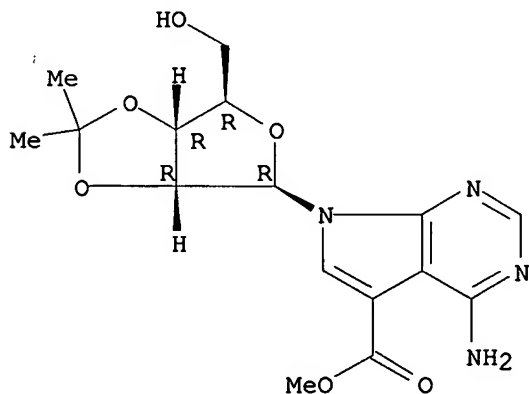
IT 50919-50-1P 50919-51-2P 50919-52-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 50919-50-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

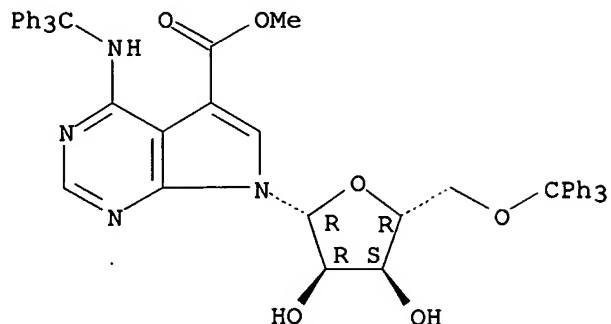
Absolute stereochemistry.



RN 50919-51-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-[(triphenylmethyl)amino]-7-[5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

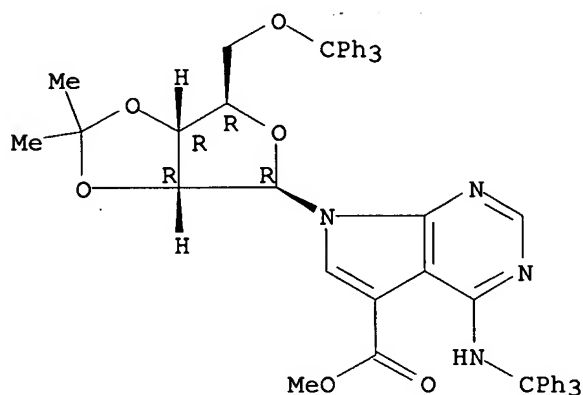
Absolute stereochemistry.



RN 50919-52-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-4-[(triphenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



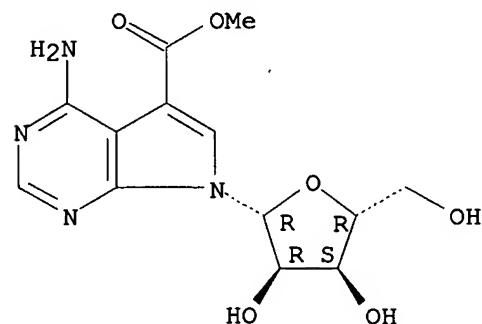
IT 18440-68-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with dimethoxypropane)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 58 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:117587 CAPLUS

DOCUMENT NUMBER: 72:117587

TITLE: Nucleoside antibiotics. VI. Biosynthesis of the  
pyrrolopyrimidine nucleoside antibiotic toyocamycin by  
Streptomyces rimosus

AUTHOR(S): Uematsu, T.; Suhadolnik, R. J.  
CORPORATE SOURCE: Dep. of Bioorg. Chem., Albert Einstein Med. Center,  
Philadelphia, PA, USA  
SOURCE: Biochemistry (1970), 9(5), 1260-6  
CODEN: BICHAW; ISSN: 0006-2960  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The biosynthesis of the pyrrolopyrimidine nucleoside antibiotic, toyocamycin, elaborated by *S. rimosus*, has been studied. Adenine-2-<sup>14</sup>C, but not adenidine-8-<sup>14</sup>C, is incorporated into toyocamycin. All of the <sup>14</sup>C in the toyocamycin from the adenine-2-<sup>14</sup>C expts. resides in C-2 of toyocamycin. This was shown by the conversion of toyocamycin into the 3-carboxyethyl derivative C-2 of toyocamycin was released as formic acid by heating 5-carboxamido-3-(2-carboxyethyl)-4-hydroxy-xy-7β-D-ribofuranosylpyrrolo[2,3-d]pyrimidine (I) in alkali. 5-Carboxy-4-hydroxy-7-(β-D-ribofuranosyl)pyrrolo[2,3 - d]pyrimidine (II), synthesized from the intermediate 2-amino-4-carboxy-3-carbonyl - [N-(2-carboxyethyl)]-1-β-D-ribofuranosylpyrrole by treatment with formic acid and Ac<sub>2</sub>O, was not radioactive. Sangivamycin, 5-carboxamido-4-hydroxy-7-(β-D - ribofuranosyl)pyrro-lo[2,3-d]pyrimidine (III), 4-hydroxypyrrolo[2,3-d]pyrimidine, I, and II were all isolated and crystallized, and their structures were rigorously characterized. The isolation of formic acid from I was unequivocally established. These data provide evidence that N-7 and C-8 of the imidazole ring of a purine are lost during the biosynthesis of the pyrrole ring of toyocamycin. III has been alkylated in good yields with β-propiolactone at N-3 of the pyrrolopyrimidine ring to form the carboxyethyl nucleoside I. This procedure affords an excellent method for opening of the pyrimidine ring and the isolation of C-2 as formic acid. The studies reported here add another role of purines in the biosynthesis of naturally occurring compds.

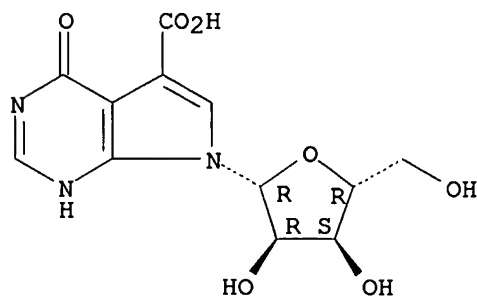
IT 28070-52-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 28070-52-2 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 59 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:413308 CAPLUS

DOCUMENT NUMBER: 71:13308

TITLE: Pyrrolopyrimidine nucleosides. III. Total synthesis of toyocamycin, sangivamycin, tubercidin, and related derivatives

AUTHOR(S): Tolman, Richard L.; Robins, Roland K.; Townsend, Leroy B.

CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA

SOURCE: Journal of the American Chemical Society (1969), 91(8), 2102-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 71:13308

GI For diagram(s), see printed CA Issue.

AB The structure of toyocamycin and sangivamycin were unequivocally established as 4-amino-5-cyano-7-( $\beta$ -D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (I) and 4-amino-5-carboxamido-7-( $\beta$ -D-ribofuranosyl)pyrrolo-[2,3-d]pyrimidine (II), resp. The total synthesis of all the presently known pyrrolo[2,3-d]pyrimidine nucleoside antibiotics (toyocamycin, sangivamycin, and tubercidin) has now been accompanied via the acid-catalyzed fusion procedure. The synthesis of several new pyrrolo[2,3-d]pyrimidine derivs. required for utilization in the fusion procedure is reported. Factors which are involved in a successful fusion reaction, e.g., the number and magnitude of electron-withdrawing substituents and the juxtaposition of these substituents in relation to the site of glycosidation, are discussed.

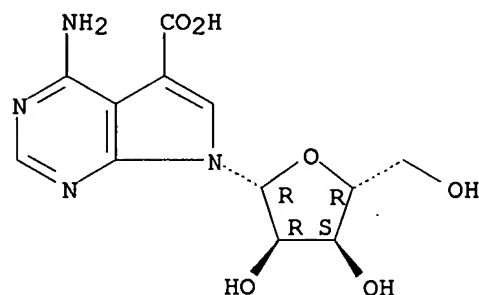
IT 18418-00-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7- $\beta$ -D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 60 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:86268 CAPLUS

DOCUMENT NUMBER: 70:86268

TITLE: Sangivamycin and derivatives

INVENTOR(S): Rao, Koppaka V.; Marsh, William S.; Renn, Donald W.

PATENT ASSIGNEE(S): Pfizer, Chas., and Co., Inc.

SOURCE: U.S., 10 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3423398	A	19690121	US 1965-454637	19650510
PRIORITY APPLN. INFO.:			US 1965-454637	A 19650510

AB Fermentation by a strain of *Streptomyces rimosus* produces sangivamycin (I), 4-amino-5-carboxamido-7-(D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine, and N-(lower alkyl) substituted amides, a deamidohydrazido derivative, N-oxide, monohydrate, and salts. All are active against tumors. Thus, a slant of *S. rimosus* ATCC 14673 was incubated for 48 hrs. at 28° in a medium of glucose 10, soy bean meal 15, distillers' solubles 2.5, K<sub>2</sub>HPO<sub>4</sub> 2, NaCl 1, and CaCO<sub>3</sub> 0.5 g./l. and propagated in the same medium with air at 1 volume/volume/min. for 72 hrs. The filtered broth was highly active against HeLa cells in tissue culture. Adsorbing on C at pH 4, eluting with 0.05N HCl in MeOH, dissolving the neutralized and dried eluate in MeOH, and passing through DEAE-cellulose gave an effluent from which I was again adsorbed, eluted, and finally crystallized from aqueous pyridine as I.H<sub>2</sub>O in rectangular prisms, m. 258-60°. The reineckate, m. 170°, also had a high inhibitory activity against tumors. Heating 2 g. I in 200 cc. 2N NaOH gave the deamido derivative of I, m. 236-8°, C<sub>12</sub>H<sub>14</sub>O<sub>6</sub>N<sub>4</sub>.HCl, its Me ester m. 216-8°, and its hydrazide 238-40°. Refluxing 0.2 g. tetraacetyl-I in 25 cc. CHCl<sub>3</sub> with 0.3

cc. POCl<sub>3</sub>, concentrating, diluting with H<sub>2</sub>O and extracting the neutralized solution with CHCl<sub>3</sub> gave tetraacetyltoycamycin, which was separated as the picrate, m. 160-2°. Treating I in AcOH with H<sub>2</sub>O<sub>2</sub> gave the N-oxide, m. 276-8°.

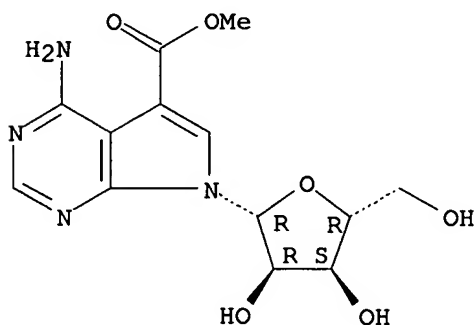
IT 18440-68-1 21090-38-0

RL: BIOL (Biological study)  
(neoplasm inhibitors)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

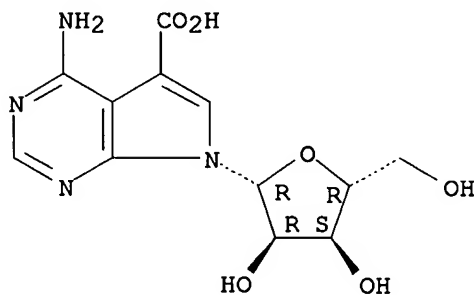
Absolute stereochemistry.



RN 21090-38-0 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L3 ANSWER 61 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:497071 CAPLUS

DOCUMENT NUMBER: 69:97071

TITLE: Structure of sangivamycin

AUTHOR(S): Rao, Koppaka V.

CORPORATE SOURCE: John L. Smith Mem. for Cancer Res., Chas. Pfizer and Co., Inc., Maywood, NJ, USA

SOURCE: Journal of Medicinal Chemistry (1968), 11(5), 939-41  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Sangivamycin (I) is an antitumor substance, a metabolite of a streptomycete culture, and shows spectral properties similar to those of nucleosides. The presence of a pentose residue was established indirectly by periodate oxidation and hydrolysis. The compound also has an aromatic amino group and a carboxamide group. Some of the similarities in properties to toycamycin (II) led to the hypothesis that sangivamycin may be closely related to this compound. This hypothesis is shown to be correct in that

sangivamycin has a carboxamide group and toyocamycin has a nitrile group on the same carbon skeleton. This relationship is established by three different methods. A brief study of the biological activity of some of the derivs. of sangivamycin is described.

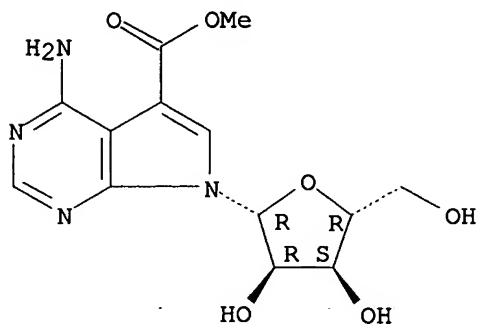
IT 18440-68-1P 21090-38-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

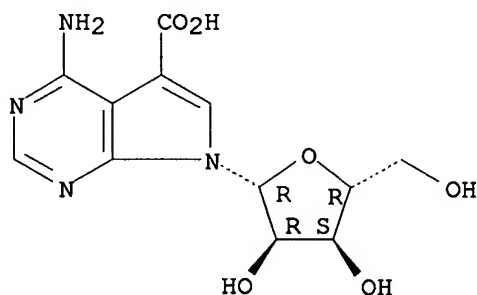
Absolute stereochemistry.



RN 21090-38-0 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L3 ANSWER 62 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:78540 CAPLUS

DOCUMENT NUMBER: 68:78540

TITLE: Pyrrolo[2,3-d]pyrimidine nucleoside antibiotics.  
Total synthesis and structure of toyocamycin, unamycin  
B, vengicide, antibiotic E-212, and sangivamycin  
(BA-90912)

AUTHOR(S): Tolman, Richard L.; Robins, Roland K.; Townsend, Leroy  
B.

CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA

SOURCE: Journal of the American Chemical Society (1968),  
90(2), 524-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 68:78540

GI For diagram(s), see printed CA Issue.

AB A total synthesis of toyocamycin (I, R = CN, R1 = H, R2 = NH2, R3 = H)  
(II) and sangivamycin (I, R = CONH2, R1 = H, R2 = NH2, R3 = H) (III) and

the unequivocal assignment of their structures are reported. Ring closure of 2-amino-5-bromo-3,4-dicyanopyrrole with formamidine acetate in EtOCH<sub>2</sub>CH<sub>2</sub>OH at reflux temperature gave 4-amino-6-bromo-5-cyanopyrrolo[2,3-d]pyrimidine (IV, R<sub>2</sub> = NH<sub>2</sub>) (IVb). IVb, Ac<sub>2</sub>O, and xylene refluxed 18 hrs. gave the monoacetylated derivative (IV, R<sub>2</sub> = NHCOMe) (IVc). IVc and tetra-O-acetyl-β-D-ribofuranose heated at 175° in the presence of bis(p-nitrophenyl) phosphate 25 min. followed by column and preparative layer chromatog. gave the acetylated nucleoside (I, R = CN, R<sub>1</sub> = Br, R<sub>2</sub> = NHCOMe, R<sub>3</sub> = Ac) (V). Treatment of V with methanolic NH<sub>3</sub> at room temperature resulted in complete deacetylation to 4-amino-6-bromo-5-cyano-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (I, R = CN, R<sub>1</sub> = Br, R<sub>2</sub> = NH<sub>2</sub>, R<sub>3</sub> = H) (VI), which was debrominated over 5% Pd-C with H to give II. A rigorous comparison of authentic samples of unamycin B, antibiotic E-212, and vengicide proved that these antibiotics are identical with II. Treatment of VI with 30% H<sub>2</sub>O<sub>2</sub> in concentrated NH<sub>4</sub>OH at room temperature gave the corresponding 5-carboxamido derivative (I, R = CONH<sub>2</sub>, R<sub>1</sub> = Br, R<sub>2</sub> = NH<sub>2</sub>, R<sub>3</sub> = H), which on debromination gave III. Addnl. evidence for the structural assignment of II and III was furnished by the conversion of sangivamycin acid to the related pyrrolo[2,3-d]pyrimidine antibiotic tubercidin (I, R = R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = NH<sub>2</sub>).

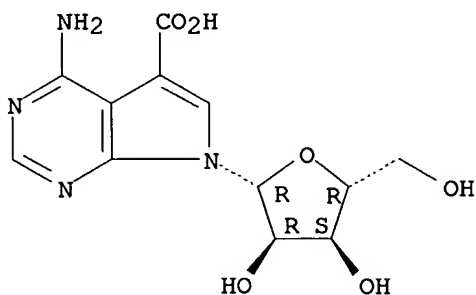
IT 18418-00-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 63 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1965:441749 CAPLUS

DOCUMENT NUMBER: 63:41749

ORIGINAL REFERENCE NO.: 63:7524e-f

TITLE: Antitumor activities and structural relation of tubercidin, toyocamycin, and their derivatives

AUTHOR(S): Saneyoshi, Mineo; Toluzen, Reiko; Fukuoka, Fumiko

CORPORATE SOURCE: Natl. Cancer Center Res. Inst., Tokyo

SOURCE: Gann (1965), 56(2), 219-22

CODEN: GANNA2; ISSN: 0016-450X

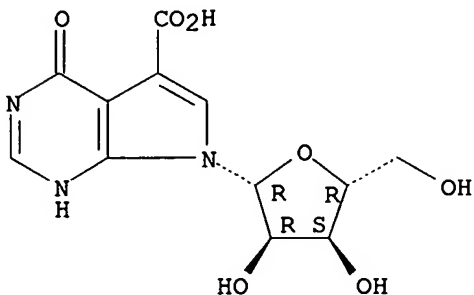
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Normal young adults of Swiss mice and Nakahara-Fukuoka sarcoma (N-F) were used. Among the compds. related to toyocamycin, the active cancericidal action in vitro depended on the coexistence of an amino group in the mol. at the 4 position, CN at the 5 position, and ribofuranose at the 7 position. When the 4 position is deaminated with HNO<sub>2</sub> (deaminohydroxytoyocamycin) the activity is markedly diminished with simultaneous decrease of toxicity. Tubercidin, is less toxic and less cancericidal than toyocamycin, and the in vitro cancericidal action is not shared by its hydroxyl derivative, deaminohydroxytubercidin. In in vivo tests, tubercidin as well as deaminohydroxytubercidin showed a slight tumor-inhibiting effect, while 4-aminopyrrolo[2,3-d]pyrimidine and 4-hydroxypyrrolo[2,3-d]pyrimidine, which are aglycons of tubercidin and deaminohydroxytubercidin, resp., are both without antitumor action and have a very low toxicity.

IT 28070-52-2, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid,  
4-hydroxy-7-β-D-ribofuranosyl-  
(as neoplasm inhibitor)  
RN 28070-52-2 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-  
D-ribofuranosyl- (9CI) (CA INDEX NAME)

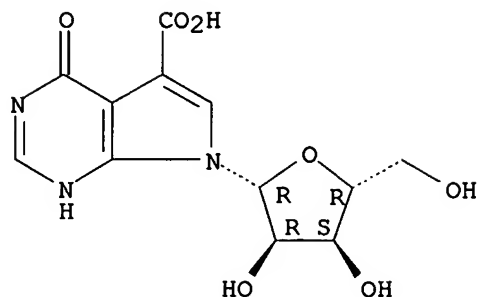
Absolute stereochemistry.



L3 ANSWER 64 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1965:441748 CAPLUS  
DOCUMENT NUMBER: 63:41748  
ORIGINAL REFERENCE NO.: 63:7524b-e  
TITLE: Pharmacological research on new acetylenic derivatives  
with hypotensive action  
AUTHOR(S): Cascio, G.; Fabra, I.; Madonia, P.; Mantia, G.; Sprio,  
V.  
CORPORATE SOURCE: Univ. Palermo, Italy  
SOURCE: Farmaco, Edizione Scientifica (1965), 20(5), 336-50  
CODEN: FRPSAX; ISSN: 0430-0920  
DOCUMENT TYPE: Journal  
LANGUAGE: Italian

AB The synthesis and pharmacol. activity of phenylacetylene derivs. are described. EtMgBr is added dropwise to an ether solution of phenylacetylene and the mixture is heated on a water bath for 1 hr., cooled, and an ether solution of acetophenone is added slowly with vigorous stirring. After 12 hrs., the solution is heated on a water bath for 2 hrs. The ether phase is separated after acidification with H<sub>2</sub>SO<sub>4</sub> to give 2,4-diphenyl-3-butyn-2-ol-1-al oxime (I) white needles, m.p. 138-40° (benzene). Similarly, 5-phenyl-3-methyl-4-pentyn-3-ol-2-one oxime (II) is prepared from isonitrosomethyl ethyl ketone as white prisms, m.p. 79° (benzene + petroleum ether). The L.D.<sub>50</sub> in the mouse is 1.250 g. I/kg., intraperitoneally, and in the rat 8.750 g./kg., orally. Corresponding values for II are 1.750 g./kg., and 3.125 g./kg., resp. In doses between 100 and 200 mg./kg., I and II show no effect on the central nervous system. I is somewhat oil soluble and shows a slight hypotensive activity. II is very soluble in oil and shows a strong and quick hypotensive effect when administered either intraparenterally or orally. By 120 min. after oral administration of 100 mg. II/kg., the arterial pressure is decreased. This decrease continues for some hrs., and then the hypotensive activity is exhausted very slowly. When the dose is 10% as large, the hypotensive activity is obtained only by a prolonged treatment. In hypotensive doses II does not modify the diuresis. II shows no ganglioplegic, sympathicolytic or parasympathicomimetic effect. By 2 hrs. after administration of a single high dose, the catechol amine levels are decreased in the blood and cerebral tissue, whereas they increase in adrenal tissue. At the end of the hypotensive effect, the catechol amine levels in blood and in brain are higher than normal, whereas in adrenal tissue they are decreased.

IT 28070-52-2, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid,  
4-hydroxy-7-β-D-ribofuranosyl-  
(as neoplasm inhibitor)  
RN 28070-52-2 CAPLUS  
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-  
D-ribofuranosyl- (9CI) (CA INDEX NAME)



L3 ANSWER 65 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1963:27298 CAPLUS

DOCUMENT NUMBER: 58:27298

ORIGINAL REFERENCE NO.: 58:4557g-h,4558a-e

TITLE: Chemical structure of toyocamycin

AUTHOR(S): Okuma, Kazuhiko

CORPORATE SOURCE: Inst. Phys. Chem. Res., Tokyo

SOURCE: J. Antibiotics (Tokyo) Ser. A (1961), 14, 343-52

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

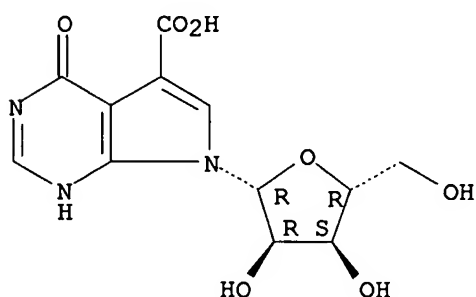
GI For diagram(s), see printed CA Issue.

AB cf. CA 55, 27330f. Streptomyces Number 1922 was cultured in a medium containing soluble starch 1.5, glucose 0.5, Polypeptone 0.5, meat extract 0.5, NaCl 0.5, K<sub>2</sub>HPO<sub>4</sub> 0.01, and soybean meal 1.0% (pH 7.0) and toyocamycin (I) was isolated from broth filtrate by adsorption on C-1 resin (salicylic acid type), elution with 80% aqueous Me<sub>2</sub>CO, concentration in vacuo, extraction with BuOH at pH 7.0, back-extraction with 0.5N HCl, and concentration in vacuo. I, C<sub>12</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub> (EtOH) or C<sub>12</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>.H<sub>2</sub>O (H<sub>2</sub>O), was colorless needles, m. 237° (decomposition) (EtOH), [α]<sub>D</sub><sup>20</sup> -45.7° (c 1.05, 0.1N HCl). I gave pos. periodate, and neg. Fehling, biuret, Pauly, FeCl<sub>3</sub>, and ninhydrin tests, was soluble in AcOH and acid, moderately soluble in MeOH, EtOH, Me<sub>2</sub>CO, dioxane, and BuOH, sparingly soluble in H<sub>2</sub>O and Et<sub>2</sub>O, and insol. in petr. ether, EtOAc, and CHCl<sub>3</sub>. I formed a monopicrate, decomposed 225-6° (H<sub>2</sub>O). I with Ac<sub>2</sub>O in C<sub>5</sub>H<sub>5</sub>N yielded a tetra-Ac derivative, m. 100°. I, heated at 70° with NaNO<sub>2</sub> in glacial AcOH, yielded a deaminohydroxy derivative of I (II), C<sub>12</sub>H<sub>12</sub>N<sub>4</sub>O<sub>5</sub>, m. 262-3°, λ 264 mμ (ε 13,870, 0.1N HCl) and 228 and 274.5 mμ (ε 12,176 and 15,330, resp., 0.1N NaOH). I consumed 1 mole of periodate without formation of HCO<sub>2</sub>H. II absorbed H on Pd-C in N HCl to yield a deaminohydroxy-decyanoaminomethyl derivative of I (III), C<sub>12</sub>H<sub>16</sub>N<sub>4</sub>O<sub>5</sub>, decomposed 246-8° (H<sub>2</sub>O), λ 260 mμ (ε 8786, 0.1N HCl), 217 and 271 mμ (ε 18,493 and 9597, resp., 0.1N NaOH), and orange yellow with ninhydrin. I refluxed in 3N HCl for 4 hrs. under N gave needles, which yielded, on deamination with NaNO<sub>2</sub> in AcOH, a deaminohydroxydecyanocarboxy derivative of I (IV), C<sub>12</sub>H<sub>15</sub>N<sub>3</sub>O<sub>6</sub>.2H<sub>2</sub>O, decomposed 278° (H<sub>2</sub>O), λ 230 and 274 mμ (ε 12,987 and 11,921, resp., 0.1N HCl), and 230 and 277 mμ (ε 9557 and 13,453, resp., 0.1N NaOH). D-Ribose was found in the hydrolyzate from I and Dowex-50 (H). II, heated at 150° in a sealed tube with HI and red P for 5 hrs., yielded 4-hydroxypyrrolo[2,3-d]pyrimidine (V), on precipitation with AgNO<sub>3</sub>, removal of Ag, and sublimation in vacuo. V, C<sub>6</sub>H<sub>5</sub>N<sub>3</sub>O, decomposed 336-40°, λ 263 mμ (ε 9650, 0.1N HCl) and 265 mμ (ε 10,300, 0.1N NaOH). V was also obtained by alkali fusion of I at 250-60° 30 min., absorption on C-1 ion exchange resin (H), elution with 80% aqueous Me<sub>2</sub>CO, chromatography on cellulose powder with BuOH-MeOH-H<sub>2</sub>O (2:1:2), concentration in vacuo, and sublimation. III was heated at 150° for 4 hrs. in a sealed tube with HI and red P, the mixture concentrated in vacuo, the insolubles in cold NH<sub>4</sub>OH warmed for 10 min. in HCl, and the filtrate was dried to 4-hydroxy-5-aminomethylpyrrolo[2,3-d]pyrimidine-HCl (VI) (decomposed above 300°), which was purified as the helianthate, C<sub>21</sub>H<sub>23</sub>N<sub>7</sub>S<sub>4</sub>, decomposed 248-50° (H<sub>2</sub>O). 4-Hydroxy-5-[bis(ethylthio)methyl]pyrrolo[2,3-d]pyrimidine (VII) was isolated by

refluxing VI in AcOH and hexamethylenetetramine 10 min., adsorbing on and eluting from C-1 ion exchange resin (H), concentrating in vacuo, and chromatographing on cellulose powder, C<sub>11</sub>H<sub>15</sub>N<sub>3</sub>S<sub>2</sub>O, decomposed 230-3°, λ 272 mμ (ε 9188, EtOH). 4-Hydroxy-5-methylpyrrolo[2,3-d]pyrimidine (VIII) was isolated by refluxing VII in 80% aqueous EtOH with Raney Ni, concentrating in vacuo, and subliming in vacuo, C<sub>7</sub>H<sub>7</sub>N<sub>3</sub>O, decomposed 280-2°, λ 225 and 273 mμ (ε 9663 and 7250, 0.1N HCl), and 271 mμ (ε 9020, 0.1N NaOH). VIII was identical with that synthesized from Et cyanoacetate via α-bromopropionaldehyde diethyl acetal, Et (α-cyano-β-methyl-γ,γ-diethoxy)butyrate, 2-mercapto-4-hydroxy-5-(1-methyl-2,2-diethoxy)-ethyl-6-aminopyrimidine, and 4-hydroxy-6-(1-methyl-2,2-diethoxy)ethyl-6-aminopyrimidine (Brit. 812,366, CA 54, 592i; Davoll, CA 54, 8840d). Thus, I [R = (D-ribofuranosyl)] was proposed as the structure of toyocamycin.

IT 89305-63-5, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-, dihydrate  
(preparation of)  
RN 89305-63-5 CAPLUS  
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-, dihydrate (7CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 H<sub>2</sub>O

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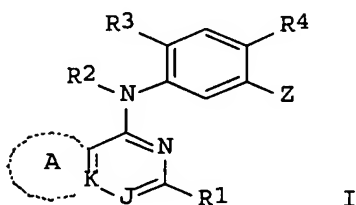
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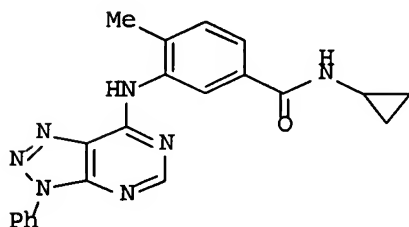
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L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:409524 CAPLUS Full-text  
 DN 142:463438  
 TI Preparation of phenylamine substituted bicyclic heterocyclic compounds  
 useful as kinase inhibitors  
 IN Das, Jagabandhu; Hynes, John; Leftheris, Katerina; Lin, Shugun; Wroblewski,  
 Stephen T.; Wu, Hong  
 PA Bristol-Myers Squibb Company, USA  
 SO PCT Int. Appl., 113 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005042537	A1	20050512	WO 2004-US35116	20041022
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	US 2005143398	A1	20050630	US 2004-970420	20041021
PRAI	US 2003-513285P	P	20031022		
OS	MARPAT 142:463438				
GI					



I



II

AB Title compds. I [J = N or CR<sub>5</sub>; R<sub>1</sub> and R<sub>5</sub> independently = H, OH, halo, CN, etc.; R<sub>2</sub> = H or alkyl; R<sub>3</sub> and R<sub>4</sub> independently = H, (un)substituted-alkyl, OH, MeO, halo, etc.; K = N or C; Z = NHR<sub>6</sub>, CONR<sub>6</sub>R<sub>7</sub>, NR<sub>6</sub>CO<sub>2</sub>R<sub>7</sub>, etc.; R<sub>6</sub> = H or (un)substituted alkyl; R<sub>7</sub> = H, OH, alkoxy, etc.; Ring A = fused heterocycle or carbocycle], and their pharmaceutically acceptable salts, prodrugs, and solvates thereof, are prepared and disclosed as kinase inhibitors. Thus, e.g., II was prepared by reaction of 4-chloro-1-phenyl- 1,2,3,5,7-azaindene

with 3-amino-4-methyl-N-cyclopropylbenzamide. I have shown activity as inhibitors of p38 $\alpha$ / $\beta$  enzymes and TNF- $\alpha$  (no data).

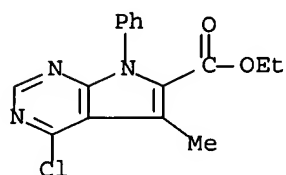
IT 245728-43-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of phenylamine substituted bicyclic heterocyclic compound as kinase inhibitors)

RN 245728-43-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-chloro-5-methyl-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2003:506580 CAPLUS Full-text  
DN 139:79178

TI Synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivatives and use as  
phosphodiesterase VII inhibitors and in combination with other agents

IN Eggenweiler, Hans-Michael; Wolf, Michael

PA Merck Patent GmbH, Germany

SO Ger. Offen., 36 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	DE 10163991	A1	20030703	DE 2001-10163991	20011224
	CA 2471538	AA	20030710	CA 2002-2471538	20021108
	WO 2003055882	A1	20030710	WO 2002-EP12533	20021108
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	EP 1458722	A1	20040922	EP 2002-805744	20021108
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	JP 2005520801	T2	20050714	JP 2003-556412	20021108
	US 2005059686	A1	20050317	US 2004-500040	20040623
	ZA 2004005859	A	20050517	ZA 2004-5859	20040722
PRAI	DE 2001-10163991	A	20011224		
	WO 2002-EP12533	W	20021108		

OS MARPAT 139:79178

AB The invention concerns the synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs.,  
their physiol. acceptable salts, stereoisomers, solvates, mixts. thereof and  
their use as phosphodiesterase VII inhibitors in the treatment of diseases  
that are influenced by the phosphodiesterase VII regulation of human  
eosinophil activation and degranulation. Osteoporosis, tumors, cachexia,  
atherosclerosis, rheumatoid arthritis, multiple sclerosis, diabetes mellitus,  
AIDS, autoimmune and heart diseases can be treated with the drugs. Thus the  
synthesis of 5-isopropyl-4-oxo-7-p-tolyl-4,7-dihydro- 3H-pyrrolo[2,3-  
d]pyrimidine-6-carboxylic acid Et ester and analog compds. is described along  
with injection, suppository, tablet and other formulations.

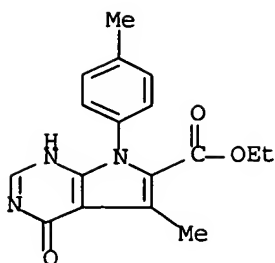
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552298-59-6P 552298-60-9P 552298-61-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs. and use as  
phosphodiesterase VII inhibitors and in combination with other agents)

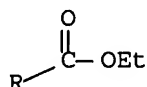
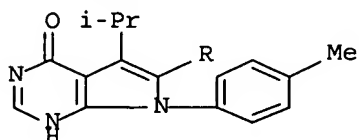
RN 120049-86-7 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-7-(4-  
methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



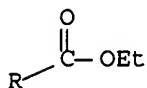
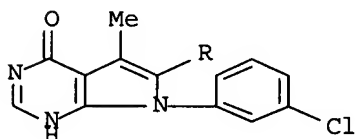
RN 552298-54-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-(1-methylethyl)-7-(4-methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



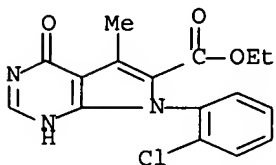
RN 552298-55-2 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(3-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



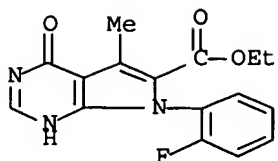
RN 552298-56-3 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



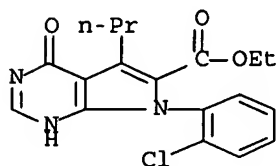
RN 552298-57-4 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-fluorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



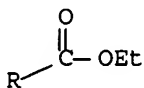
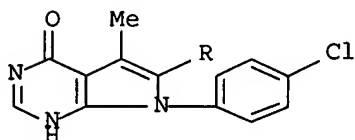
RN 552298-58-5 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-4-oxo-5-propyl-, ethyl ester (9CI) (CA INDEX NAME)



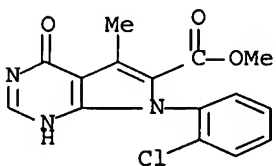
RN 552298-59-6 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(4-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



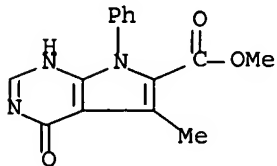
RN 552298-60-9 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

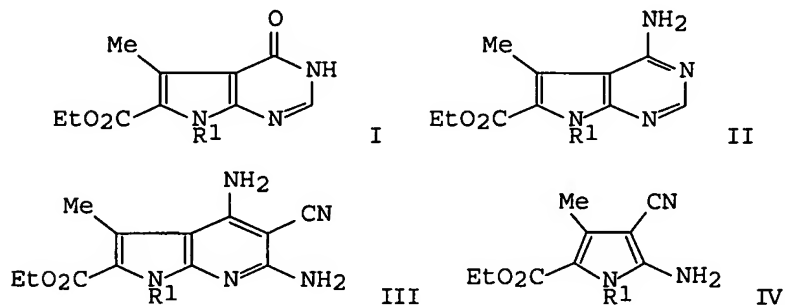


RN 552298-61-0 CAPLUS

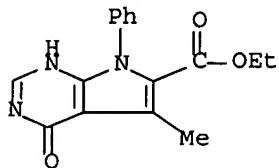
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-phenyl-, methyl ester (9CI) (CA INDEX NAME)



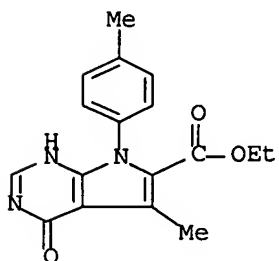
L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1989:173185 CAPLUS Full-text  
 DN 110:173185  
 TI Reactions with heterocyclic enaminonitriles. Synthesis of  
 pyrrolo[2,3-b]pyridine, pyrrolo[2,3-d]pyrimidine and pyrrole derivatives  
 AU Abdelhamid, Abdou O.; Abdel-Galil, Fathy M.; Saleh, Sohair S.  
 CS Fac. Sci., Cairo Univ., Giza, Egypt  
 SO Heterocycles (1988), 27(8), 1861-6  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DT Journal  
 LA English  
 OS CASREACT 110:173185  
 GI



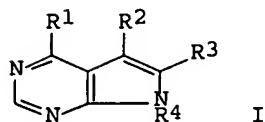
AB Pyrrolopyrimidines I and II and pyrrolopyridines III ( $R_1$  = Ph, tolyl) were prepared from aminopyrrolecarbonitriles IV. IV were heated with aqueous  $\text{HCO}_2\text{H}$  to give I. The reaction of IV with  $\text{HCONH}_2$ ,  $\text{HCO}_2\text{H}$ , and DMF gave II. III were prepared from IV and  $\text{CH}_2(\text{CN})_2$ ; IV and  $\text{NCCH}_2\text{CO}_2\text{Et}$  also gave pyrrolopyridines.  
 IT 120049-85-6P 120049-86-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 120049-85-6 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



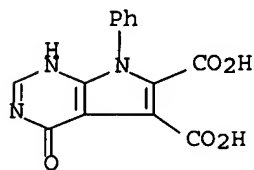
RN 120049-86-7 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-7-(4-methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



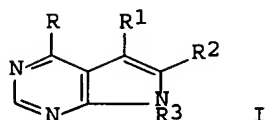
L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1987:43451 CAPLUS Full-text  
 DN 106:43451  
 TI Receptor affinity of xanthine oxidase inhibitors: structural requirements. An example of computer-assisted drug design (CADD) and molecular modeling  
 AU Folkers, Gerd  
 CS Pharm. Inst., Univ. Tuebingen, Tuebingen, 7400, Fed. Rep. Ger.  
 SO Deutsche Apotheker Zeitung (1986), 126(41), 2243-7  
 CODEN: DAZEAA2; ISSN: 0011-9857  
 DT Journal  
 LA German  
 GI



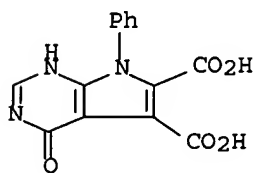
AB Structure-activity relations for pyrrolopyrimidines (I; R1 = NH2, OH; R2 = R3 = CO2H, CHO, or Me; R4 = iso-Pr or Ph) as inhibitors of xanthine oxidase (XOD) [9002-17-9] were studied by using computer-assisted drug design and mol. modeling. The inhibition of XOD by I(R1 = NH2; R2 = R3 = CO2H; R4 = Ph) [101153-20-2] and I(R1 = OH; R2 = R3 = CO2H; R4 = Ph [ 101153-21-3]) was substituent dependent. The tautomeric capability of the pyrimidine portion of I was an essential feature for the interaction of I with the enzyme receptor.  
 IT 101153-21-3  
 RL: BIOL (Biological study)  
 (xanthine oxidase inhibition by, structure in relation to)  
 RN 101153-21-3 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5,6-dicarboxylic acid, 4,7-dihydro-4-oxo-7-phenyl- (9CI) (CA INDEX NAME)



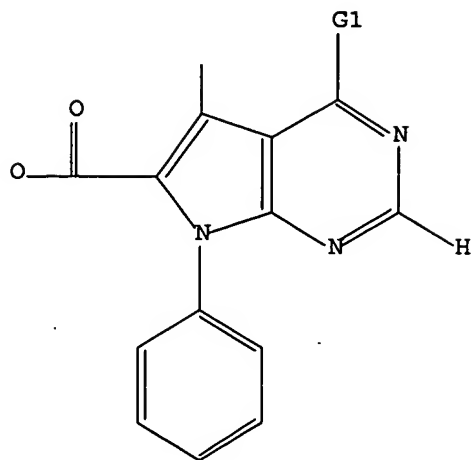
L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1986:141712 CAPLUS Full-text  
 DN 104:141712  
 TI Active site molecular modeling of xanthine oxidase inhibitors with  
 antiinflammatory activity  
 AU Folkers, Gerd; Hoeltje, Hans Dieter  
 CS Pharm. Inst., Univ. Berne, Bern, CH-3012, Switz.  
 SO Journal of Molecular Graphics (1985), 3(4), 146-50  
 CODEN: JMGRDV; ISSN: 0263-7855  
 DT Journal  
 LA English  
 GI



AB QSAR in the interaction of antiinflammatory pyrrolopyrimidines (I; R = OH or NH<sub>2</sub>; R<sub>1</sub> and R<sub>2</sub> = CO<sub>2</sub>H, Me, or CHO; R<sub>3</sub> = iso-Pr or Ph) with the active site of xanthine oxidase [9002-17-9] were examined with the use of e MO and quantum mol. mech. methods. The results explain the active site preference and decreasing inhibitory potency of the Me, CHO, and CO<sub>2</sub>H derivs.  
 IT 101153-21-3  
 RL: BIOL (Biological study)  
 (xanthine oxidase inhibition by, QSAR in)  
 RN 101153-21-3 CAPLUS  
 CN 1H-Pyrrolo[2,3-d]pyrimidine-5,6-dicarboxylic acid, 4,7-dihydro-4-oxo-7-phenyl- (9CI) (CA INDEX NAME)



=> d l2; d his; log y  
L2 HAS NO ANSWERS  
L1 STR



G1 X,O

Structure attributes must be viewed using STN Express query preparation.  
L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 08:34:09 ON 04 MAY 2006)

FILE 'REGISTRY' ENTERED AT 08:34:16 ON 04 MAY 2006

L1 STRUCTURE UPLOADED  
L2 QUE L1  
L3 1 S L2  
L4 12 S L2 FUL

FILE 'CAPLUS' ENTERED AT 08:35:32 ON 04 MAY 2006

L5 5 S L4

FILE 'STNGUIDE' ENTERED AT 08:36:09 ON 04 MAY 2006

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.06	193.66
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.75

STN INTERNATIONAL LOGOFF AT 08:36:16 ON 04 MAY 2006